```
=> fil reg
FILE 'REGISTRY' ENTERED AT 15:09:12 ON 07 JUL 2001
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STRUCTURE FILE UPDATES:     6 JUL 2001  HIGHEST RN 344832-24-2
DICTIONARY FILE UPDATES:    6 JUL 2001  HIGHEST RN 344832-24-2

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Structure search limits have been increased.  See HELP SLIMIT
for details.

=> d sta que l43
L6          124 SEA FILE=REGISTRY ABB=ON  PLU=ON  (108-40-7/BI OR 110-91-8/BI
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                19
L12             STR
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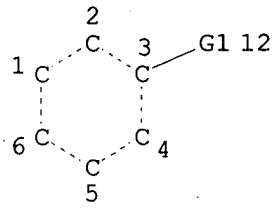
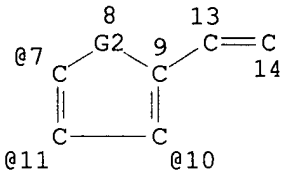
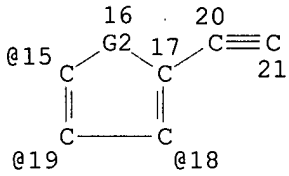
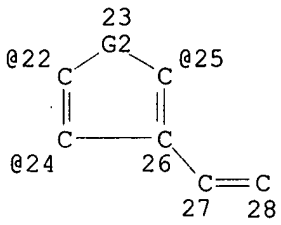
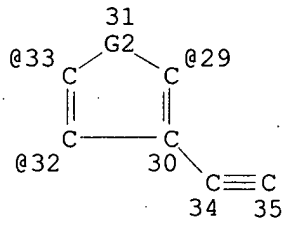
Point of Contact:
Jan Delaval
Librarian-Physical Sciences
CM1 1E01 Tel: 308-4498

VAR G1=7/11/10/15/19/18/22/24/25/33/32/29
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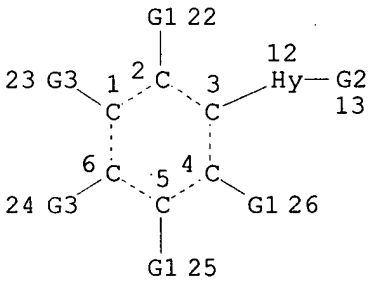
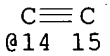
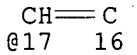
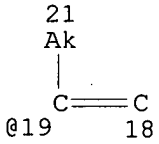
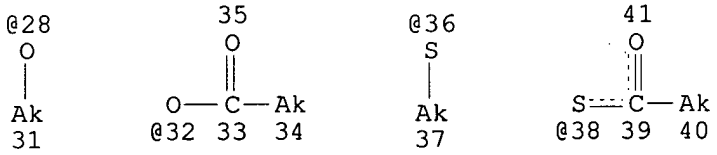
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE
L14 4061 SEA FILE=REGISTRY SSS FUL L12
L17 STR

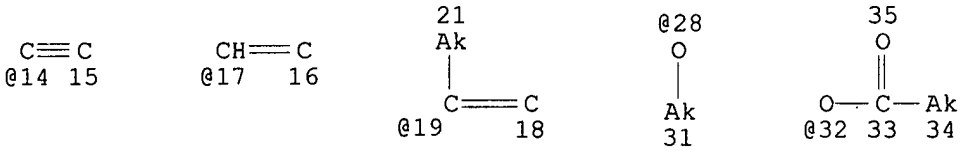






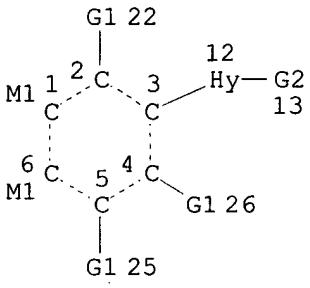
VAR G1=H/X/AK/OH/28/32
VAR G2=14/17/19
VAR G3=H/AK/OH/28/32/SH/36/38
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 15
CONNECT IS M1 RC AT 16
CONNECT IS M1 RC AT 18
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY AT 12
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1
NUMBER OF NODES IS 32

STEREO ATTRIBUTES: NONE
L19 1007 SEA FILE=REGISTRY SUB=L14 CSS FUL L17
L25 STR

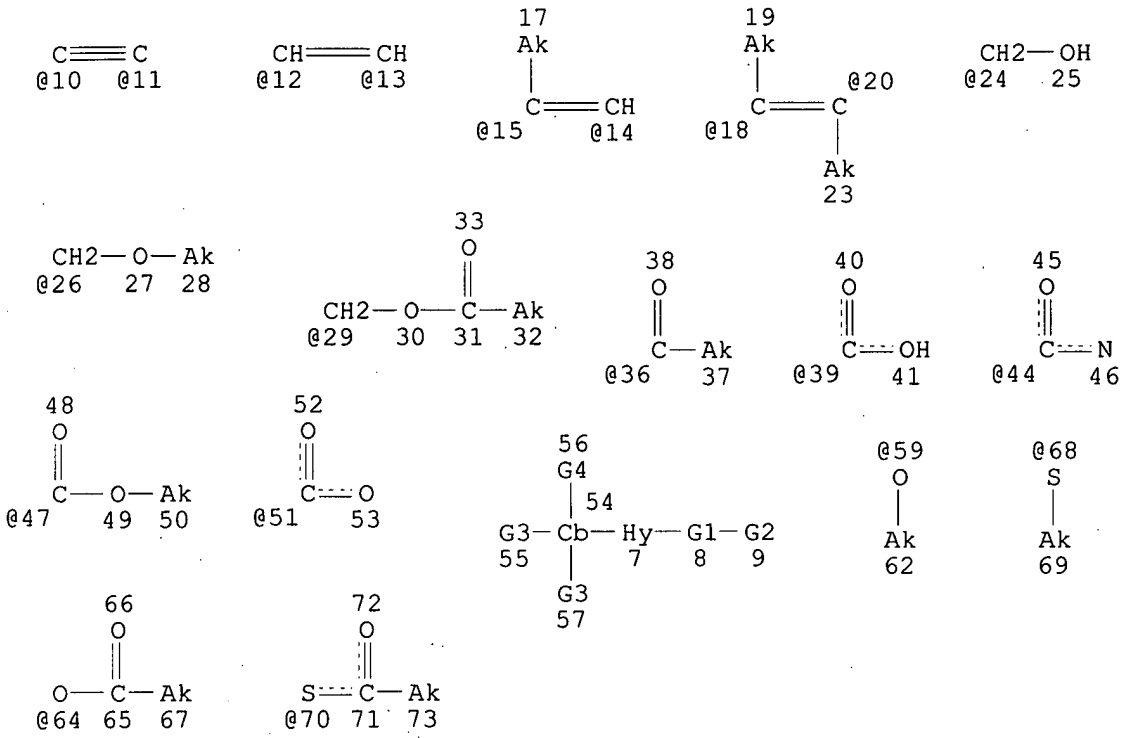




VAR G1=H/X/AK/OH/28/32
VAR G2=14/17/19
NODE ATTRIBUTES:
HCOUNT IS M1 AT 1
HCOUNT IS M1 AT 6
CONNECT IS M1 RC AT 15
CONNECT IS M1 RC AT 16
CONNECT IS M1 RC AT 18
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY AT 12
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 2
NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE
L26 734 SEA FILE=REGISTRY SUB=L19 SSS FUL L25
L27 273 SEA FILE=REGISTRY ABB=ON PLU=ON L19 NOT L26
L28 STR



VAR G1=10-7 11-9/12-7 13-9/15-7 14-9/14-7 15-9/18-7 20-9
VAR G2=AK/24/26/29/CHO/36/39/44/47/51
VAR G3=H/AK/OH/59/64/SH/68/70
VAR G4=H/X/AK/OH/59/64
NODE ATTRIBUTES:
NSPEC IS RC AT 46
CONNECT IS M1 RC AT 46
CONNECT IS M1 RC AT 50
CONNECT IS M1 RC AT 53
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY AT 7
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 56

STEREO ATTRIBUTES: NONE

L30 43 SEA FILE=REGISTRY SUB=L27 CSS FUL L28
L31 15 SEA FILE=REGISTRY ABB=ON PLU=ON L6 AND L14
L33 7 SEA FILE=REGISTRY ABB=ON PLU=ON L31 AND L19
L34 6 SEA FILE=REGISTRY ABB=ON PLU=ON L33 NOT BR/ELS
L35 38 SEA FILE=REGISTRY ABB=ON PLU=ON L30 NOT L31
L36 17 SEA FILE=REGISTRY ABB=ON PLU=ON L35 AND (C14H12O4 OR C14H12O3 OR C29H34N2O2S OR C15H14O4 OR C29H34NO2PS OR C16H16O2S OR C14H12O4 OR C18H20O2S OR C28H32NO2PS OR C18H20O3S OR C30H37N2O2S OR C17H18O2S)
L37 4 SEA FILE=REGISTRY ABB=ON PLU=ON L36 AND C14H12O3
L38 1 SEA FILE=REGISTRY ABB=ON PLU=ON L37 NOT METHYLPHENYL
L39 13 SEA FILE=REGISTRY ABB=ON PLU=ON L36 NOT L37
L40 20 SEA FILE=REGISTRY ABB=ON PLU=ON (L39 OR L38 OR L34)
L41 24 SEA FILE=REGISTRY ABB=ON PLU=ON L30 NOT L40
L42 1 SEA FILE=REGISTRY ABB=ON PLU=ON L41 AND C30H36N2O2S
L43 21 SEA FILE=REGISTRY ABB=ON PLU=ON (L40 OR L42)

=> d his

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     (FILE 'HOME' ENTERED AT 14:05:20 ON 07 JUL 2001)
                SET COST OFF

     FILE 'HCAPLUS' ENTERED AT 14:05:28 ON 07 JUL 2001
                E BERNARDON J/AU
L1           62 S E4-E7
                E WO98-FR391/AP,PRN
                E WO97-FR391/AP,PRN
L2            1 S E3,E4
                E FR96-3235/AP,PRN
L3            1 S E3,E4
L4            1 S L2,L3
L5            1 S L1 AND L4
                SEL RN

     FILE 'REGISTRY' ENTERED AT 14:07:03 ON 07 JUL 2001
L6          124 S E1-E124
L7           16 S L6 AND (46.150.18 AND (16.138.5 OR 16.145.3))/RID
L8           16 S L6 AND (C6 AND (OC4 OR SC4))/ES
L9           16 S L7,L8
L10             STR
L11          50 S L10
L12             STR L10
L13          50 S L12
L14        4061 S L12 FUL
                SAV L14 QAZI619/A
L15             STR
L16          20 S L15 CSS SAM SUB=L14
L17             STR L10
L18          45 S L17 CSS SAM SUB=L14
L19        1007 S L17 CSS FUL SUB=L14
                SAV L19 QAZI691A/A
L20             STR L15
L21          18 S L20 SAM SUB=L19

     FILE 'HCAOLD' ENTERED AT 14:37:41 ON 07 JUL 2001
L22          12 S L19

     FILE 'REGISTRY' ENTERED AT 14:37:53 ON 07 JUL 2001
L23          11 S L19 AND CAOLD/LC
L24         996 S L19 NOT L23
L25             STR L17
L26         734 S L25 FUL SUB=L19
L27         273 S L19 NOT L26
                SAV L26 QAZI691B/A
L28             STR L15
L29           3 S L28 CSS SAM SUB=L27
L30          43 S L28 CSS FUL SUB=L27
                SAV L30 QAZI691C/A
L31          15 S L6 AND L14
L32           9 S L9 NOT L14
L33           7 S L31 AND L19
L34           6 S L33 NOT BR/ELS
L35          38 S L30 NOT L31
L36          17 S L35 AND (C14H12O4 OR C14H12O3 OR C29H34N2O2S OR C15H14O4 OR C
L37           4 S L36 AND C14H12O3
L38           1 S L37 NOT METHYLPHENYL
L39          13 S L36 NOT L37
L40          20 S L39,L38,L34
L41          24 S L30 NOT L40
L42           1 S L41 AND C30H36N2O2S
L43          21 S L40,L42
L44         228 S L27 NOT L29-L43
                SAV L43 QAZI691D/A
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     FILE 'HCAPLUS' ENTERED AT 15:08:18 ON 07 JUL 2001
L45           10 S L43
L46            1 S L45 AND L1-L5
L47            9 S L45 AND (PY<=1997 OR PRY<=1997 OR AY<=1997)
L48           10 S L45-L47

     FILE 'USPATFULL' ENTERED AT 15:09:01 ON 07 JUL 2001
L49            3 S L45

     FILE 'REGISTRY' ENTERED AT 15:09:12 ON 07 JUL 2001

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 15:09:21 ON 07 JUL 2001
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FILE COVERS 1947 - 7 Jul 2001  VOL 135 ISS 3
FILE LAST UPDATED: 6 Jul 2001  (20010706/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

 This file supports REG1stRY for direct browsing and searching of
 all substance data from the REGISTRY file.  Enter HELP FIRST for
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in CA from 1947 to the present.  On April 22, 2001, bibliographic
information and abstracts were added for over 2.2 million references
published in CA from 1947 to 1966.


=> d l48 all hitstr tot

L48  ANSWER 1 OF 10  HCAPLUS  COPYRIGHT 2001 ACS
AN   1999:455007  HCAPLUS
DN   131:194472
TI   Quantitative structure-activity relationship studies of RAR .alpha.,
     .beta., .gamma. retinoid agonists
AU   Douguet, Dominique; Thoreau, Etienne; Grassy, Gerard
CS   Centre International Recherches Dermatologie GALDERMA, Sophia Antipolis,
     F-06902, Fr.
SO   Quant. Struct.-Act. Relat. (1999), 18(2), 107-123
     CODEN: QSARDI; ISSN: 0931-8771
PB   Wiley-VCH Verlag GmbH
DT   Journal
LA   English
CC   2-2 (Mammalian Hormones)
AB   Structure-activity relationships were established for 140 synthetic
     retinoid agonists.  Retinoids, natural and synthetic analogs of vitamin A,
     are activating ligands for retinoic acid receptors (RAR.alpha., .beta.,
     and .gamma.), members of the nuclear receptor superfamily.  A QSAR study
     provides information on the type of intermol. and intramol. interactions
     the active mols. are exposed to during the course of their interaction
     with the receptor.  Retinoid structures were modeled both by mol. and
     quantum mechanics and were submitted to a preliminary conformational anal.
     based on mol. dynamics.  Linear and non-linear multivariate analyses were
     performed, revealing the principal electronic and structural
     characteristics leading to good affinity for each RAR subtype.  Distinct
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structural features were found for each subtype: this is in agreement with the fact that the selectivity of the RAR subtypes results from the change of amino acids in the ligand cavity. Indeed, these amino-acids induce subtle changes in terms of steric properties and specific interactions, thus engendering specificity. The predictive ability of these relationships was validated using a large set of compds. which were not used to derive the model. The goal this of work was to detect relationships between structures and affinity for a broad range of retinoids in order that this model could be used in a more general manner, for example to impose constraints in database searching, or for use in automatic structure generation software.

ST retinoid structure activity relationship mol modeling; retinoic acid receptor QSAR

IT Drug design
Molecular modeling
QSAR (structure-activity relationship)
(QSAR studies of retinoic acid receptors .alpha., .beta., .gamma. retinoid agonists)

IT Retinoic acid receptors
Retinoids
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR studies of retinoic acid receptors .alpha., .beta., .gamma. retinoid agonists)

IT Retinoic acid receptors
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(RAR-.alpha.; QSAR studies of retinoic acid receptors .alpha., .beta., .gamma. retinoid agonists)

IT Retinoic acid receptors
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(RAR-.beta.; QSAR studies of retinoic acid receptors .alpha., .beta., .gamma. retinoid agonists)

IT Retinoic acid receptors
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(RAR-.gamma.; QSAR studies of retinoic acid receptors .alpha., .beta., .gamma. retinoid agonists)

IT 71441-28-6, Ttnpb 86471-16-1 94497-51-5, AM 80 99660-54-5
99660-64-7 102121-60-8, Am580 104224-10-4 104224-38-6 104224-43-3
104249-87-8 106685-40-9, Cd 271 106685-58-9 107430-51-3, Cd 0367
107430-66-0 107430-70-6 107430-75-1 110368-35-9 110952-17-5
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118292-41-4 119435-88-0 119435-89-1 119567-97-4 119568-07-9
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241140-19-2 241140-20-5 241140-21-6 241140-23-8 241140-24-9
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241140-34-1 241140-35-2 241140-36-3
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR studies of retinoic acid receptors .alpha., .beta., .gamma. retinoid agonists)

RE.CNT 77
RE

(1) Abraham, R; J Computer Aided Mol Design 1989, V3, P175 HCAPLUS
(2) Amstrong, R; The Retinoids Biology, Chemistry and Medicine 1994, P545
(3) Anon; JP 06072866 HCAPLUS
(4) Bernardon, J; WO 92/06948 1991 HCAPLUS
(5) Bernardon, J; EP 0661258 A1 1994 HCAPLUS
(6) Bernardon, J; EP 0661260 A1 1994 HCAPLUS
(7) Bernardon, J; EP 0679630 A1 1995 HCAPLUS
(8) Bernardon, J; EP 0679631 A1 1995 HCAPLUS
(9) Bernardon, J; EP 0722928 A1 1995 HCAPLUS
(10) Bernardon, J; EP 0776881 A1 1996 HCAPLUS
(11) Bernardon, J; WO 97/33856 1996 HCAPLUS
(12) Bernardon, J; WO 97/33881 1997 HCAPLUS
(13) Bernardon, J; Patent deposed 1998
(14) Boehm, M; J Med Chem 1994, V37, P2930 HCAPLUS
(15) Bonchev, D; J Med Chem 1993, V36, P1562 HCAPLUS
(16) Bonchev, D; J Med Chem 1994, V37, P2300 HCAPLUS
(17) Boyd, A; Am J Med 1989, V86, P568 MEDLINE
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(19) Carbo, R; Int J Quantum Chem 1987, V32, P517 HCAPLUS
(20) Cavey, M; Anal Biochem 1990, V186, P19 HCAPLUS
(21) Chambon, P; The Faseb J 1996, V10, P940 HCAPLUS
(22) Chandraratna, R; EP 0284288 1988 HCAPLUS
(23) Chandraratna, R; EP 0337689 1989 HCAPLUS
(24) Chandraratna, R; US 5602130 1993 HCAPLUS
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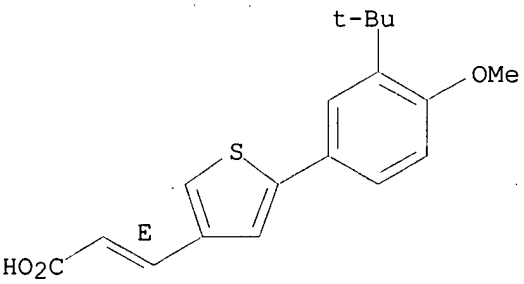
IT **241140-32-9 241140-33-0**
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR studies of retinoic acid receptors .alpha., .beta., .gamma. retinoid agonists)

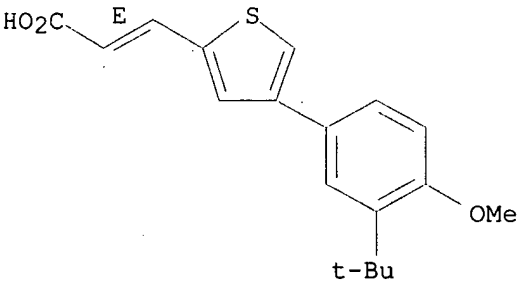
RN 241140-32-9 HCAPLUS
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 241140-33-0 HCAPLUS
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L48 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2001 ACS
AN 1999:421672 HCAPLUS
DN 131:73571
TI Preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compounds as MCP-1 receptor

antagonists.
IN Shiraishi, Mitsuru; Kitayoshi, Takahito; Aramaki, Yoshio; Honda, Susumu; Oda, Tsuneo
PA Takeda Chemical Industries, Ltd., Japan
SO PCT Int. Appl., 513 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D295-12
ICS A61K031-16; A61K031-33; A61K031-66; C07C233-62; C07D213-20; C07D213-61; C07D213-84; C07D213-85; C07F009-44; C07F009-54; C07F009-6584; C07F009-6568; C07F009-655; C07F009-53; C07D313-08; C07D407-12
CC 27-21 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 25, 63
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9932468	A1	19990701	WO 1998-JP5707	19981217 <--
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RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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AU 9916830	A1	19990712	AU 1999-16830	19981217 <--
EP 1040103	A1	20001004	EP 1998-961383	19981217 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
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JP 11263764	A2	19990928	JP 1998-360780	19981218 <--
NO 2000003133	A	20000809	NO 2000-3133	20000616 <--
PRAI JP 1997-351481	A	19971219 <--		
WO 1998-JP5707	W	19981217		

OS MARPAT 131:73571
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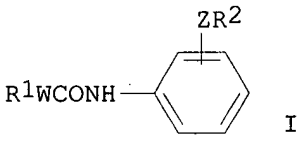

I

AB Title compds. I [R1 = (substituted) 5-6 membered ring; W = Q1, Q2; A = atoms to form a (substituted) 5-6 membered arom. ring; X = S, O, (substituted) C, N; B = atoms to form a (substituted) 5-7 membered ring; Z = bond, divalent group; R2 = (substituted) amino, ammonio, heterocyclyl, S-bonded group, P(O)kR5R6; k = 0, 1; R5, R6 = (substituted) hydrocarbyl, amino; PR5R6 = cyclic group], were prepd. Thus, 7-(4-methylphenyl)-2,3-dihydro-1-benzoxepine-4-carboxylic acid in CH2Cl2 was treated with (COCl)2 and DMF to give a residue which was stirred with 4-[N-methyl-N-(tetrahydropyran-4-yl)aminomethyl]aniline and Et3N in THF to give N-[4-[N-methyl-N-(tetrahydropyran-4-yl)aminomethyl]phenyl]-7-(4-methylphenyl)-2,3-dihydro-1-benzoxepine-4-carboxamide (II). II at 1 .mu.M inhibited MCP-1 induced chemotaxis in CHO cells by 89%. A II capsule

compn. is given.

ST benzoxepinecarboxamide prepn monocyte chemoattractant protein receptor antagonist; benzocycloheptenecarboxamide prepn monocyte chemoattractant protein receptor antagonist; naphthalenecarboxamide prepn monocyte chemoattractant protein receptor antagonist; myocarditis treatment benzoxepinecarboxamide benzocycloheptenecarboxamide naphthalenecarboxamide; cardiac infarction treatment benzoxepinecarboxamide benzocycloheptenecarboxamide naphthalenecarboxamide

IT Monocyte chemoattractant protein-1
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(antagonists; prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Heart, disease
(infarction, treatment; prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Cytokine receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(monocyte chemoattractant protein-1; prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Heart, disease
(myocarditis, treatment; prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Monocyte chemoattractant protein-1
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(receptors; prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 229003-88-7P 229004-17-5P 229004-21-1P
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 229003-36-5P 229003-37-6P 229003-38-7P 229003-39-8P 229003-40-1P
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229005-69-0P 229005-70-3P 229005-71-4P 229005-72-5P 229005-73-6P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 229005-74-7P 229005-75-8P 229005-76-9P 229005-77-0P 229005-78-1P
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RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 75-64-9, tert-Butylamine, reactions 76-05-1, reactions 78-67-1
96-22-0, 3-Pentanone 96-97-9 98-53-3, 4-tert-Butylcyclohexanone
99-98-9, 4-Dimethylaminoaniline 100-11-8, 4-Nitrobenzylbromide
100-14-1, 4-Nitrobenzylchloride 100-48-1, 4-Cyanopyridine 100-54-9,
3-Cyanopyridine 100-60-7, N-Cyclohexyl-N-methylamine 100-61-8,
N-Methylaniline, reactions 100-76-5, Quinuclidine 102-69-2,
Tripropylamine 103-67-3, N-Methylbenzylamine 103-76-4,
1-(2-Hydroxyethyl)piperazine 106-41-2, 4-Bromophenol 106-53-6,
4-Bromothiophenol 107-08-4 107-15-3, 1,2-Ethanediamine, reactions
108-94-1, Cyclohexanone, reactions 108-99-6, 3-Picoline 109-01-3,
1-Methylpiperazine 109-04-6, 2-Bromopyridine 109-06-8, 2-Picoline
110-52-1, 1,4-Dibromobutane 110-68-9, N-Methyl-N-butylamine 110-87-2
110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions
111-24-0, 1,5-Dibromopentane 111-33-1 111-42-2, reactions 111-49-9

111-96-6, Bis(2-methoxyethyl)ether 120-92-3, Cyclopentanone 121-44-8, reactions 122-00-9 123-75-1, Pyrrolidine, reactions 123-90-0, Thiomorpholine 288-47-1, Thiazole 358-23-6, Trifluoromethanesulfonic acid anhydride 407-14-7, 4-Trifluoromethoxybromobenzene 462-08-8, 3-Aminopyridine 497-38-1, Norcamphor 502-42-1, Cycloheptanone 534-03-2, 2-Amino-1,3-propanediol 536-78-7, 3-Ethylpyridine 539-88-8, Ethyl levulinate 555-16-8, 4-Nitrobenzaldehyde, reactions 585-70-6, 5-Bromo-2-furancarboxylic acid 588-96-5, 4-Bromophenetole 591-22-0, 3,5-Lutidine 591-49-1, 1-Methylcyclohexene 616-44-4 617-05-0, Ethyl vanillate 617-27-6 619-23-8, 3-Nitrobenzyl chloride 619-73-8, 4-Nitrobenzylalcohol 620-87-1, 2-(4-Nitrobenzyl)pyridine 625-43-4, N-Methylisobutylamine 626-60-8, 3-Chloropyridine 626-67-5, 1-Methylpiperidine 765-58-2, 5-Bromo-2-methylthiophene 766-09-6, 1-Ethylpiperidine 766-97-2, 4-Methylphenylacetylene 771-99-3, 4-Phenylpiperidine 841-77-0, 1-Benzhydrylpiperazine 930-69-8, Sodium phenylsulfide 998-40-3, Tributylphosphine 1003-09-4, 2-Bromothiophene 1072-72-6, 4H-Tetrahydrothiopyran-4-one 1080-32-6, Diethyl benzylphosphonate 1121-92-2 1205-62-5, 4-Nitrobenzylphosphonic acid 1450-75-5 1484-84-0, 2-(2-Hydroxyethyl)piperidine 1585-07-5, 4-Ethylbromobenzene 1663-39-4 1679-18-1, 4-Chlorophenylboronic acid 1692-15-5 1722-12-9, 2-Chloropyrimidine 1761-61-1, 5-Bromosalicylaldehyde 1765-93-1, 4-Fluorophenylboronic acid 2320-30-1, 3,5-Dimethylcyclohexanone 2338-18-3 2605-67-6 2635-13-4 2969-81-5, Ethyl-4-bromobutyrate 3132-99-8, 3-Bromobenzaldehyde 3218-02-8, Amino-methylcyclohexane 3287-99-8, Benzylamine hydrochloride 3433-37-2, 2-Piperidinemethanol 3490-06-0 3492-64-6 4068-76-2, Methyl-5-bromosalicylate 4606-65-9, 3-(Hydroxymethyl)piperidine 4701-17-1, 5-Bromo-2-thiophenecarboxaldehyde 4746-97-8, 1,4-Cyclohexanedione monoethyleneketal 5105-78-2 5205-39-0 5332-73-0, 3-Methoxypropylamine 5339-26-4, 4-(2-Bromoethyl)nitrobenzene 5382-16-1, 4-Hydroxypiperidine 5459-93-8, N-Ethylcyclohexylamine 5466-06-8, Ethyl 3-mercaptopropionate 5720-05-8, 4-Methylphenylboronic acid 5794-88-7, 5-Bromoanthranilic acid 6165-69-1 6291-85-6, 3-Ethoxypropylamine 6388-74-5, p-Nitrostyreneoxide 6602-32-0, 2-Bromo-3-hydroxypyridine 6638-79-5, N,O-Dimethylhydroxylamine hydrochloride 6836-19-7, 7-Methoxy-1-tetralone 6850-65-3, 4-Aminocyclohexanol 6859-99-0, 3-Hydroxypiperidine 10544-63-5, Ethyl crotonate 13331-23-2, 2-Furylboronic acid 13331-27-6, 3-Nitrophenylboronic acid 13515-93-0, Sarcosine methyl ester hydrochloride 13623-25-1, 6-Methoxy-1-indanone 13952-84-6, 1-Methylpropylamine 15300-97-7 16419-60-6 17857-14-6, (3-Carboxypropyl)triphenylphosphonium bromide 18471-73-3, 2-(4-Aminophenyl)pyridine 18600-42-5, p-Nitrobenzylamine hydrochloride 18664-32-9, 1,3-Dimethoxyacetone 18791-75-8, 4-Bromo-2-thiophenecarboxaldehyde 20074-79-7, Diethyl 4-aminobenzylphosphonate 20826-04-4, 5-Bromonicotinic acid 20980-22-7, 1-(2-Pyrimidyl)piperazine 23462-75-1, Tetrahydropyran-3-one 24252-37-7, Ethyl 1-methylpiperidine-4-carboxylate 25808-30-4 28611-39-4 29943-42-8, 4H-Tetrahydropyran-4-one 31252-42-3, 4-Benzylpiperidine 32231-06-4, 1-(3,4-Methylenedioxybenzyl)-piperazine 35386-24-4, 1-(2-Methoxyphenyl)piperazine 38212-30-5, 1-(4-Methoxyphenyl)piperazine 50541-93-0, 4-Amino-1-benzylpiperidine 50729-68-5 52146-35-7, 1-(3,4,5-Trimethoxybenzyl)piperazine 60548-09-6, 1-(2-Furoyl)piperazine hydrochloride 61081-32-1 73579-08-5, 1-Methyl-4-methylaminopiperidine 79099-07-3 80670-21-9 82261-42-5, 3-(4-Aminophenyl)pyridine 85199-06-0 87779-78-0 89878-14-8, Diethyl-(3-pyridyl)-borane 93777-26-5, 5-Bromo-2-fluorobenzaldehyde 96251-92-2 98546-51-1, 4-Methylthiophenylboronic acid 128796-39-4, 4-Trifluoromethylphenylboronic acid 162210-31-3 162271-10-5 175394-06-6 186498-02-2 229009-38-5 229009-39-6 229009-40-9 229009-41-0 229009-42-1 229009-43-2
RL: RCT (Reactant)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 623-04-1P, 4-Aminobenzyl alcohol 955-44-2P 2089-33-0P 2439-56-7P

4519-78-2P, Benzyldiethylphosphine oxide 5339-15-1P 6149-46-8P
6406-74-2P 6425-46-3P 6763-91-3P 6881-57-8P, Benzylphosphonic acid
14473-91-7P 15084-55-6P 15115-76-1P 15184-96-0P 16341-77-8P
17302-46-4P 18483-99-3P 18484-05-4P 20173-88-0P 20712-12-3P
22009-38-7P, 7-Hydroxy-1-tetralone 22237-13-4P, 4-Ethoxyphenylboronic
acid 24100-18-3P 29124-57-0P 29608-05-7P 34035-05-7P 34160-40-2P
38035-10-8P 40594-34-1P 41526-73-2P, 7-Phenyl-1-tetralone
42870-65-5P 50534-23-1P 50534-24-2P 51013-67-3P 53678-61-8P
54306-15-9P 55008-98-5P 55009-03-5P 55580-07-9P 55580-08-0P
56851-32-2P 58498-12-7P 59507-44-7P 59507-46-9P 59719-62-9P
62157-62-4P 62803-47-8P, 6-Hydroxy-1-indanone 62806-32-0P
63139-21-9P, 4-Ethylphenylboronic acid 73676-23-0P 79432-87-4P
79909-21-0P 83619-74-3P 91150-58-2P 91953-92-3P 92033-77-7P
93138-55-7P 94839-07-3P 95323-86-7P 98008-66-3P 123324-71-0P,
4-tert-Butylphenylboronic acid 131230-76-7P 133851-67-9P
135605-97-9P 138007-25-7P 139301-27-2P, 4-
Trifluoromethoxyphenylboronic acid 142335-64-6P 143632-57-9P
144464-65-3P 145654-38-2P 147539-41-1P 160127-63-9P 162607-15-0P
162607-20-7P 168897-21-0P 175393-25-6P 175394-17-9P 175840-02-5P
179055-22-2P 183608-47-1P 185111-27-7P 229006-54-6P 229006-55-7P
229006-56-8P 229006-57-9P 229006-58-0P 229006-59-1P 229006-60-4P
229006-61-5P 229006-62-6P 229006-63-7P 229006-64-8P 229006-65-9P
229006-66-0P 229006-67-1P 229006-68-2P 229006-69-3P 229006-70-6P
229006-71-7P 229006-72-8P 229006-73-9P 229006-74-0P 229006-75-1P
229006-76-2P 229006-77-3P 229006-78-4P 229006-79-5P 229006-80-8P
229006-81-9P 229006-82-0P 229006-83-1P 229006-84-2P 229006-85-3P
229006-86-4P 229006-87-5P 229006-88-6P 229006-89-7P 229006-90-0P
229006-91-1P 229006-92-2P 229006-93-3P 229006-94-4P 229006-95-5P
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229007-11-8P 229007-12-9P 229007-13-0P 229007-14-1P 229007-15-2P
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229007-51-6P 229007-52-7P 229007-53-8P 229007-54-9P 229007-55-0P
229007-56-1P 229007-57-2P 229007-58-3P 229007-59-4P 229007-60-7P
229007-61-8P 229007-62-9P 229007-63-0P 229007-64-1P 229007-65-2P
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229007-76-5P 229007-77-6P 229007-78-7P 229007-79-8P 229007-80-1P
229007-81-2P 229007-82-3P 229007-83-4P 229007-84-5P 229007-85-6P
229007-86-7P 229007-87-8P 229007-88-9P 229007-89-0P 229007-90-3P
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229008-06-4P 229008-07-5P 229008-09-7P 229008-11-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides,
naphthalenecarboxamides, and related compds. as MCP-1 receptor
antagonists)

IT 229008-14-4P 229008-16-6P 229008-18-8P 229008-20-2P 229008-22-4P
229008-24-6P 229008-26-8P 229008-27-9P 229008-28-0P 229008-29-1P
229008-30-4P 229008-31-5P 229008-32-6P 229008-33-7P 229008-34-8P
229008-35-9P 229008-36-0P 229008-37-1P 229008-38-2P 229008-39-3P
229008-40-6P 229008-41-7P 229008-42-8P 229008-43-9P 229008-44-0P
229008-45-1P 229008-46-2P 229008-47-3P 229008-48-4P 229008-49-5P
229008-50-8P 229008-51-9P 229008-52-0P 229008-53-1P
229008-54-2P 229008-55-3P 229008-56-4P
229008-57-5P 229008-58-6P 229008-59-7P 229008-60-0P
229008-61-1P 229008-62-2P 229008-63-3P 229008-64-4P 229008-65-5P
229008-66-6P 229008-67-7P 229008-68-8P 229008-69-9P 229008-70-2P

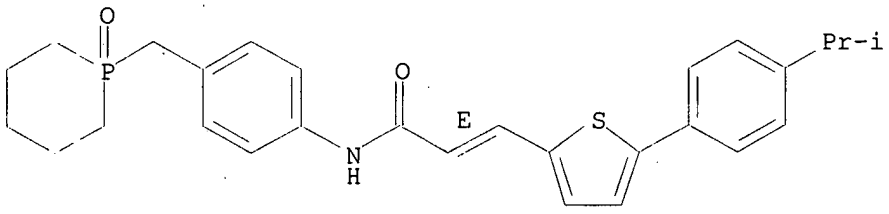
229008-71-3P 229008-72-4P 229008-73-5P 229008-74-6P 229008-75-7P
229008-76-8P 229008-77-9P 229008-78-0P 229008-79-1P 229008-80-4P
229008-81-5P 229008-82-6P 229008-83-7P 229008-84-8P 229008-85-9P
229008-86-0P 229008-87-1P 229008-88-2P 229008-89-3P 229008-90-6P
229008-91-7P 229008-92-8P 229008-93-9P 229008-94-0P 229008-95-1P
229008-96-2P 229008-97-3P 229008-98-4P 229008-99-5P 229009-00-1P
229009-01-2P 229009-02-3P 229009-03-4P 229009-04-5P 229009-05-6P
229009-06-7P 229009-07-8P 229009-08-9P 229009-09-0P 229009-10-3P
229009-11-4P 229009-12-5P 229009-13-6P 229009-14-7P 229009-15-8P
229009-16-9P 229009-17-0P 229009-18-1P 229009-19-2P 229009-20-5P
229009-21-6P 229009-22-7P 229009-23-8P 229009-24-9P 229009-25-0P
229009-26-1P 229009-27-2P 229009-28-3P 229009-29-4P 229009-30-7P
229009-31-8P 229009-32-9P 229009-33-0P 229009-34-1P 229009-35-2P
229009-36-3P 229009-37-4P 229153-66-6P 229153-67-7P 229153-68-8P
229153-69-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

RE.CNT 2
RE
(1) Teijin Ltd; JP 07025756 A 1995 HCAPLUS
(2) Teijin Ltd; JP 07025757 A 1995 HCAPLUS

IT **229006-01-3P 229006-02-4P 229006-06-8P**
229006-08-0P 229006-12-6P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

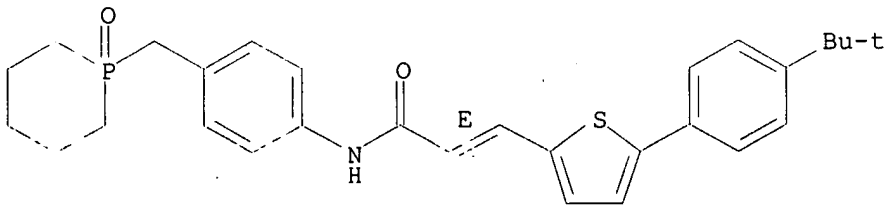
RN 229006-01-3 HCAPLUS
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229006-02-4 HCAPLUS
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

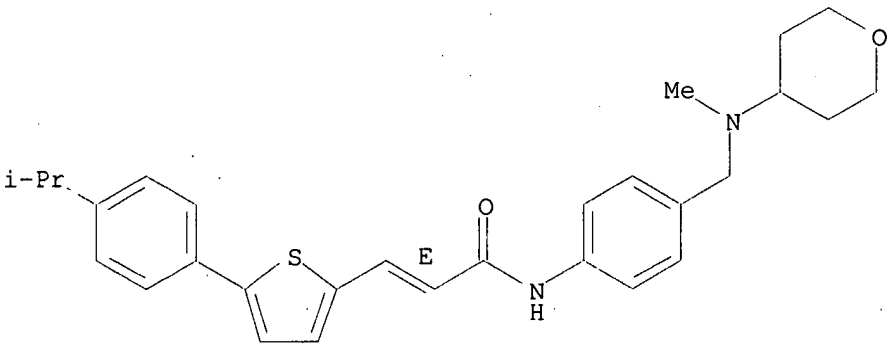
Double bond geometry as shown.



RN 229006-06-8 HCAPLUS
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA

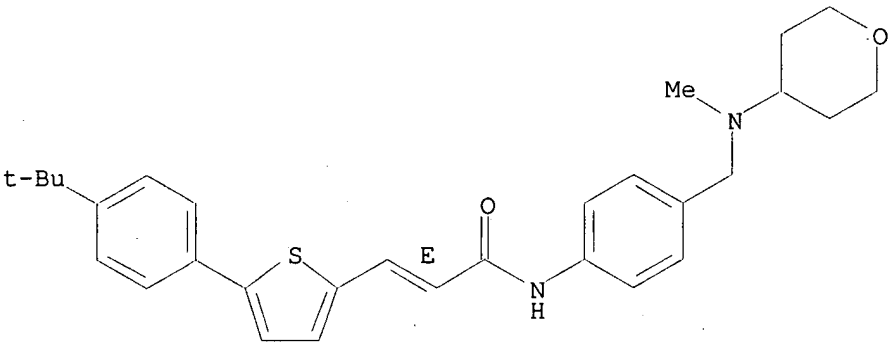
INDEX NAME)

Double bond geometry as shown.



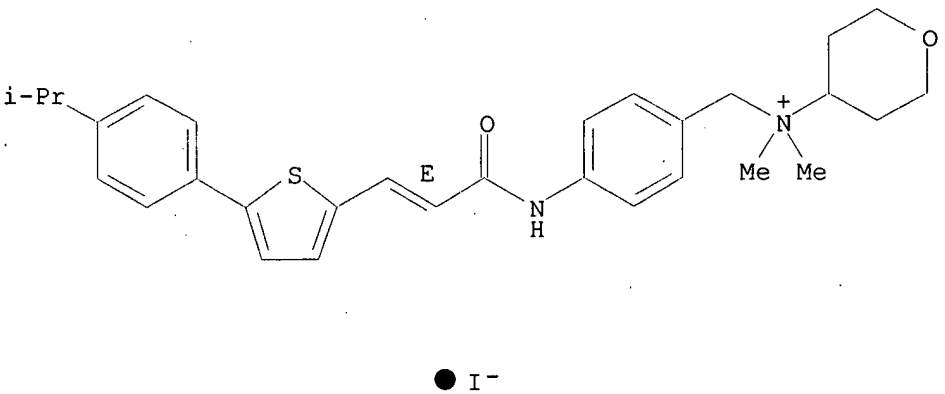
RN 229006-08-0 HCAPLUS
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229006-12-6 HCAPLUS
CN 2H-Pyran-4-aminium, tetrahydro-N,N-dimethyl-N-[[4-[[(2E)-3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-1-oxo-2-propenyl]amino]phenyl]methyl]-, iodide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

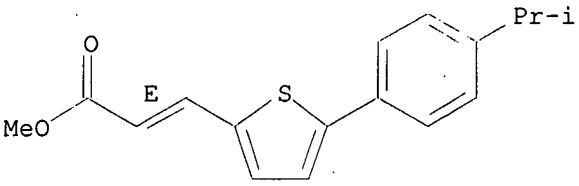


IT **229008-54-2P 229008-55-3P 229008-56-4P**
229008-57-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides,

naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

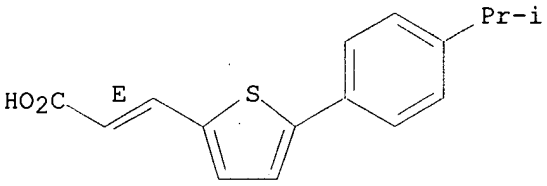
RN 229008-54-2 HCAPLUS
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



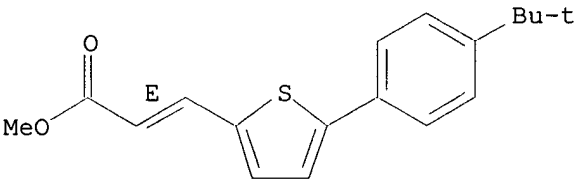
RN 229008-55-3 HCAPLUS
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



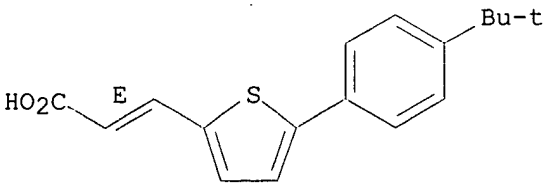
RN 229008-56-4 HCAPLUS
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229008-57-5 HCAPLUS
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L48 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2001 ACS
AN 1999:421562 HCAPLUS
DN 131:87834

TI Preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compounds as CCR5 antagonists.

IN Nishimura, Osamu; Baba, Masanori; Sawada, Hidekazu; Kanzaki, Naoyuki; Kuroshima, Ken-ichi; Shiraishi, Mitsuru; Aramaki, Yoshio
PA Takeda Chemical Industries, Ltd., Japan

SO PCT Int. Appl., 516 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K031-00
CC 27-21 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 25, 63

FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9932100	A2	19990701	WO 1998-JP5708	19981217 <--
WO 9932100	A3	19990910		
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AU 9916831	A1	19990712	AU 1999-16831	19981217 <--
EP 1039899	A2	20001004	EP 1998-961384	19981217 <--
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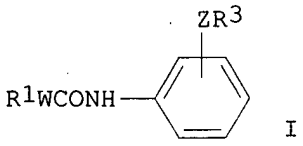
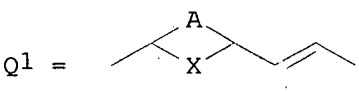
BR 9813691	A	20001010	BR 1998-13691	19981217 <--
JP 2000128782	A2	20000509	JP 1998-360820	19981218 <--
US 6096780	A	20000801	US 1999-377040	19990819
NO 2000003179	A	20000619	NO 2000-3179	20000619 <--

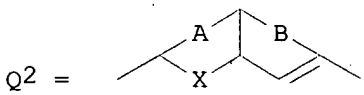
PRAI JP 1997-351480 A 19971219 <--
JP 1998-218875 A 19980803
JP 1998-234388 A 19980820
JP 1998-234398 A 19980820
US 1998-104845 P 19981016
WO 1998-JP5708 W 19981217

OS MARPAT 131:87834
GI



I





AB A pharmaceutical compn. for antagonizing CCR5 comprises I [R1 = (substituted) 5-6 membered ring; W = Q1, Q2; A = atoms to form a (substituted) 5-6 membered arom. ring; X = S, O, (substituted) C, N; B = atoms to form a (substituted) 5-7 membered ring; Z = bond, divalent group; R2 = (substituted) amino, ammonio, heterocyclyl, S-bonded group, P(O)kR5R6; k = 0, 1; R5, R6 = (substituted) hydrocarbyl, amino; PR5R6 = cyclic group]. Thus, 7-(4-methylphenyl)-2,3-dihydro-1-benzoxepine-4-carboxylic acid in CH2Cl2 was treated with (COCl)2 and DMF to give a residue which was stirred with 4-[N-methyl-N-(tetrahydropyran-4-

yl)aminomethyl]aniline and Et3N in THF to give N-[4-[N-methyl-N-(tetrahydropyran-4-yl)aminomethyl]phenyl]-7-(4-methylphenyl)-2,3-dihydro-1-benzoxepine-4-carboxamide (II). A II capsule compn. is given.

ST benzoxepinecarboxamide prepn chemokine coreceptor antagonist; benzocycloheptenecarboxamide prepn chemokine coreceptor antagonist; naphthalenecarboxamide prepn chemokine coreceptor antagonist; AIDS treatment benzoxepinecarboxamide benzocycloheptenecarboxamide naphthalenecarboxamide

IT Monocyte chemoattractant protein-1
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(antagonists; prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Cytokine receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(monocyte chemoattractant protein-1; prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Anti-AIDS agents
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Monocyte chemoattractant protein-1
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(receptors; prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Cytokine receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(.beta. chemokine receptor CCR5; prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Chemokines
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(.beta., receptor CCR5; prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 229003-88-7P 229004-17-5P 229004-21-1P
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 229003-36-5P 229003-37-6P 229003-38-7P 229003-39-8P 229003-40-1P
229003-41-2P 229003-42-3P 229003-43-4P 229003-44-5P 229003-45-6P
229003-46-7P 229003-47-8P 229003-48-9P 229003-49-0P 229003-50-3P
229003-51-4P 229003-52-5P 229003-53-6P 229003-54-7P 229003-55-8P
229003-56-9P 229003-57-0P 229003-58-1P 229003-59-2P 229003-60-5P
229003-61-6P 229003-62-7P 229003-63-8P 229003-64-9P 229003-65-0P
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229003-71-8P 229003-72-9P 229003-73-0P 229003-74-1P 229003-75-2P
229003-76-3P 229003-77-4P 229003-78-5P 229003-79-6P 229003-80-9P
229003-81-0P 229003-82-1P 229003-83-2P 229003-84-3P 229003-85-4P
229003-86-5P 229003-87-6P 229003-89-8P 229003-90-1P 229003-91-2P
229003-92-3P 229003-93-4P 229003-94-5P 229003-95-6P 229003-96-7P
229003-97-8P 229003-98-9P 229003-99-0P 229004-00-6P 229004-01-7P
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229004-12-0P 229004-13-1P 229004-14-2P 229004-15-3P 229004-16-4P
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229004-59-5P 229004-60-8P 229004-61-9P 229004-62-0P 229004-63-1P
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229005-39-4P 229005-40-7P 229005-41-8P 229005-42-9P 229005-43-0P
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229005-59-8P 229005-60-1P 229005-61-2P 229005-62-3P 229005-63-4P
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229005-69-0P 229005-70-3P 229005-71-4P 229005-72-5P 229005-73-6P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 229005-74-7P 229005-75-8P 229005-76-9P 229005-77-0P 229005-78-1P
229005-79-2P 229005-80-5P 229005-81-6P 229005-82-7P 229005-83-8P
229005-84-9P 229005-85-0P 229005-86-1P 229005-87-2P 229005-88-3P
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229005-94-1P 229005-95-2P 229005-96-3P 229005-97-4P 229005-98-5P
229005-99-6P 229006-00-2P **229006-01-3P** **229006-02-4P**
229006-03-5P 229006-04-6P 229006-05-7P **229006-06-8P**
229006-07-9P **229006-08-0P** 229006-09-1P 229006-10-4P
229006-11-5P **229006-12-6P** 229006-13-7P 229006-14-8P
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229006-45-5P 229006-46-6P 229006-47-7P 229006-48-8P 229006-49-9P
229006-50-2P 229006-51-3P 229006-52-4P 229006-53-5P 229009-44-3P
229009-45-4P 229009-46-5P 229009-47-6P 229153-64-4P 229153-65-5P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 75-64-9, tert-Butylamine, reactions 76-05-1, reactions 78-67-1
96-22-0, 3-Pentanone 96-97-9 98-53-3, 4-tert-Butylcyclohexanone
99-98-9, 4-Dimethylaminoaniline 100-11-8, 4-Nitrobenzylbromide
100-14-1, 4-Nitrobenzylchloride 100-48-1, 4-Cyanopyridine 100-54-9,
3-Cyanopyridine 100-60-7, N-Cyclohexyl-N-methylamine 100-61-8,
N-Methylaniline, reactions 100-76-5, Quinuclidine 102-69-2,

Tripropylamine 103-67-3, N-Methylbenzylamine 103-76-4, 1-(2-Hydroxyethyl)piperazine 106-41-2, 4-Bromophenol 106-53-6, 4-Bromothiophenol 107-08-4 107-15-3, 1,2-Ethanediamine, reactions 108-94-1, Cyclohexanone, reactions 108-99-6, 3-Picoline 109-01-3, 1-Methylpiperazine 109-04-6, 2-Bromopyridine 109-06-8, 2-Picoline 110-52-1, 1,4-Dibromobutane 110-68-9, N-Methyl-N-butylamine 110-87-2 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 111-24-0, 1,5-Dibromopentane 111-33-1 111-42-2, reactions 111-49-9 111-96-6, Bis(2-methoxyethyl)ether 120-92-3, Cyclopentanone 121-44-8, reactions 122-00-9 123-75-1, Pyrrolidine, reactions 123-90-0, Thiomorpholine 288-47-1, Thiazole 358-23-6, Trifluoromethanesulfonic acid anhydride 407-14-7, 4-Trifluoromethoxybromobenzene 462-08-8, 3-Aminopyridine 497-38-1, Norcamphor 502-42-1, Cycloheptanone 534-03-2, 2-Amino-1,3-propanediol 536-78-7, 3-Ethylpyridine 539-88-8, Ethyl levulinate 555-16-8, 4-Nitrobenzaldehyde, reactions 585-70-6, 5-Bromo-2-furancarboxylic acid 588-96-5, 4-Bromophenetole 591-22-0, 3,5-Lutidine 591-49-1, 1-Methylcyclohexene 616-44-4 617-05-0, Ethyl vanillate 617-27-6 619-23-8, 3-Nitrobenzyl chloride 619-73-8, 4-Nitrobenzylalcohol 620-87-1, 2-(4-Nitrobenzyl)pyridine 625-43-4, N-Methylisobutylamine 626-60-8, 3-Chloropyridine 626-67-5, 1-Methylpiperidine 765-58-2, 5-Bromo-2-methylthiophene 766-09-6, 1-Ethylpiperidine 766-97-2, 4-Methylphenylacetylene 771-99-3, 4-Phenylpiperidine 841-77-0, 1-Benzhydrylpiperazine 930-69-8, Sodium phenylsulfide 998-40-3, Tributylphosphine 1003-09-4, 2-Bromothiophene 1072-72-6, 4H-Tetrahydrothiopyran-4-one 1080-32-6, Diethyl benzylphosphonate 1121-92-2 1205-62-5, 4-Nitrobenzylphosphonic acid 1450-75-5 1484-84-0, 2-(2-Hydroxyethyl)piperidine 1585-07-5, 4-Ethylbromobenzene 1663-39-4 1679-18-1, 4-Chlorophenylboronic acid 1692-15-5 1722-12-9, 2-Chloropyrimidine 1761-61-1, 5-Bromosalicylaldehyde 1765-93-1, 4-Fluorophenylboronic acid 2320-30-1, 3,5-Dimethylcyclohexanone 2338-18-3 2605-67-6 2635-13-4 2969-81-5, Ethyl-4-bromobutyrate 3132-99-8, 3-Bromobenzaldehyde 3218-02-8, Amino-methylcyclohexane 3287-99-8, Benzylamine hydrochloride 3433-37-2, 2-Piperidinemethanol 3490-06-0 3492-64-6 4068-76-2, Methyl-5-bromosalicylate 4606-65-9, 3-(Hydroxymethyl)piperidine 4701-17-1, 5-Bromo-2-thiophenecarboxaldehyde 4746-97-8, 1,4-Cyclohexanedione monoethyleneketal 5105-78-2 5205-39-0 5332-73-0, 3-Methoxypropylamine 5339-26-4, 4-(2-Bromoethyl)nitrobenzene 5382-16-1, 4-Hydroxypiperidine 5459-93-8, N-Ethylcyclohexylamine 5466-06-8, Ethyl 3-mercaptopropionate 5720-05-8, 4-Methylphenylboronic acid 5794-88-7, 5-Bromoanthranilic acid 6165-69-1 6291-85-6, 3-Ethoxypropylamine 6388-74-5, p-Nitrostyreneoxide 6602-32-0, 2-Bromo-3-hydroxypyridine 6638-79-5, N,O-Dimethylhydroxylamine hydrochloride 6836-19-7, 7-Methoxy-1-tetralone 6850-65-3, 4-Aminocyclohexanol 6859-99-0, 3-Hydroxypiperidine 10544-63-5, Ethyl crotonate 13331-23-2, 2-Furylboronic acid 13331-27-6, 3-Nitrophenylboronic acid 13515-93-0, Sarcosine methyl ester hydrochloride 13623-25-1, 6-Methoxy-1-indanone 13952-84-6, 1-Methylpropylamine 15300-97-7 16419-60-6 17857-14-6, (3-Carboxypropyl)triphenylphosphonium bromide 18471-73-3, 2-(4-Aminophenyl)pyridine 18600-42-5, p-Nitrobenzylamine hydrochloride 18664-32-9, 1,3-Dimethoxyacetone 18791-75-8, 4-Bromo-2-thiophenecarboxaldehyde 20074-79-7, Diethyl 4-aminobenzylphosphonate 20826-04-4, 5-Bromonicotinic acid 20980-22-7, 1-(2-Pyrimidyl)piperazine 23462-75-1, Tetrahydropyran-3-one 24252-37-7, Ethyl 1-methylpiperidine-4-carboxylate 25808-30-4 28611-39-4 29943-42-8, 4H-Tetrahydropyran-4-one 31252-42-3, 4-Benzylpiperidine 32231-06-4, 1-(3,4-Methylenedioxybenzyl)-piperazine 35386-24-4, 1-(2-Methoxyphenyl)piperazine 38212-30-5, 1-(4-Methoxyphenyl)piperazine 50541-93-0, 4-Amino-1-benzylpiperidine 50729-68-5 52146-35-7, 1-(3,4,5-Trimethoxybenzyl)piperazine 60548-09-6, 1-(2-Furoyl)piperazine hydrochloride 61081-32-1 73579-08-5, 1-Methyl-4-methylaminopiperidine 79099-07-3 80670-21-9 82261-42-5, 3-(4-Aminophenyl)pyridine 85199-06-0 87779-78-0 89878-14-8, Diethyl-(3-pyridyl)-borane 93777-26-5, 5-Bromo-2-fluorobenzaldehyde 96251-92-2 98546-51-1, 4-Methylthiophenylboronic acid 128796-39-4, 4-

Trifluoromethylphenylboronic acid 162210-31-3 162271-10-5
175394-06-6 186498-02-2 229009-38-5 229009-39-6 229009-40-9
229009-41-0 229009-42-1 229009-43-2
RL: RCT (Reactant)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 623-04-1P, 4-Aminobenzyl alcohol 955-44-2P 2089-33-0P 2439-56-7P
4519-78-2P, Benzyldiethylphosphine oxide 5339-15-1P 6149-46-8P
6406-74-2P 6425-46-3P 6763-91-3P 6881-57-8P, Benzylphosphonic acid
14473-91-7P 15084-55-6P 15115-76-1P 15184-96-0P 16341-77-8P
17302-46-4P 18483-99-3P 18484-05-4P 20173-88-0P 20712-12-3P
22009-38-7P, 7-Hydroxy-1-tetralone 22237-13-4P, 4-Ethoxyphenylboronic acid 24100-18-3P 29124-57-0P 29608-05-7P 34035-05-7P 34160-40-2P
38035-10-8P 40594-34-1P 41526-73-2P, 7-Phenyl-1-tetralone
42870-65-5P 50534-23-1P 50534-24-2P 51013-67-3P 53678-61-8P
54306-15-9P 55008-98-5P 55009-03-5P 55580-07-9P 55580-08-0P
56851-32-2P 58498-12-7P 59507-44-7P 59507-46-9P 59719-62-9P
62157-62-4P 62803-47-8P, 6-Hydroxy-1-indanone 62806-32-0P
63139-21-9P, 4-Ethylphenylboronic acid 73676-23-0P 79432-87-4P
79909-21-0P 83619-74-3P 91150-58-2P 91953-92-3P 92033-77-7P
93138-55-7P 94839-07-3P 95323-86-7P 98008-66-3P 123324-71-0P,
4-tert-Butylphenylboronic acid 131230-76-7P 133851-67-9P
135605-97-9P 138007-25-7P 139301-27-2P, 4-
Trifluoromethoxyphenylboronic acid 142335-64-6P 143632-57-9P
144464-65-3P 145654-38-2P 147539-41-1P 160127-63-9P 162607-15-0P
162607-20-7P 168897-21-0P 175393-25-6P 175394-17-9P 175840-02-5P
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229007-36-7P 229007-37-8P 229007-38-9P 229007-39-0P 229007-40-3P
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229007-66-3P 229007-67-4P 229007-68-5P 229007-69-6P 229007-70-9P
229007-71-0P 229007-72-1P 229007-73-2P 229007-74-3P 229007-75-4P
229007-76-5P 229007-77-6P 229007-78-7P 229007-79-8P 229007-80-1P
229007-81-2P 229007-82-3P 229007-83-4P 229007-84-5P 229007-85-6P
229007-86-7P 229007-87-8P 229007-88-9P 229007-89-0P 229007-90-3P
229007-91-4P 229007-92-5P 229007-93-6P 229007-94-7P 229007-95-8P
229007-96-9P 229007-97-0P 229007-98-1P 229007-99-2P 229008-00-8P
229008-01-9P 229008-02-0P 229008-03-1P 229008-04-2P 229008-05-3P
229008-06-4P 229008-07-5P 229008-09-7P 229008-11-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 229008-14-4P 229008-16-6P 229008-18-8P 229008-20-2P 229008-22-4P
229008-24-6P 229008-26-8P 229008-27-9P 229008-28-0P 229008-29-1P
229008-30-4P 229008-31-5P 229008-32-6P 229008-33-7P 229008-34-8P

229008-35-9P 229008-36-0P 229008-37-1P 229008-38-2P 229008-39-3P
229008-40-6P 229008-41-7P 229008-42-8P 229008-43-9P 229008-44-0P
229008-45-1P 229008-46-2P 229008-47-3P 229008-48-4P 229008-49-5P
229008-50-8P 229008-51-9P 229008-52-0P 229008-53-1P
229008-54-2P 229008-55-3P 229008-56-4P
229008-57-5P 229008-58-6P 229008-59-7P 229008-60-0P
229008-61-1P 229008-62-2P 229008-63-3P 229008-64-4P 229008-65-5P
229008-66-6P 229008-67-7P 229008-68-8P 229008-69-9P 229008-70-2P
229008-71-3P 229008-72-4P 229008-73-5P 229008-74-6P 229008-75-7P
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229008-81-5P 229008-82-6P 229008-83-7P 229008-84-8P 229008-85-9P
229008-86-0P 229008-87-1P 229008-88-2P 229008-89-3P 229008-90-6P
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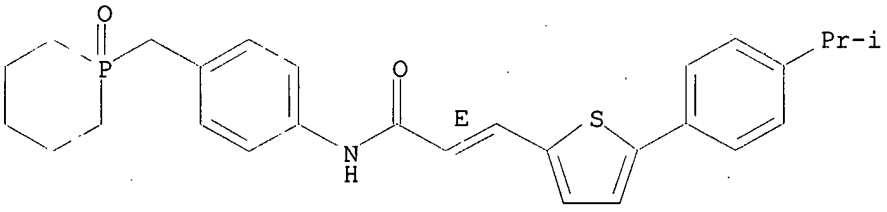
229009-16-9P 229009-17-0P 229009-18-1P 229009-19-2P 229009-20-5P
229009-21-6P 229009-22-7P 229009-23-8P 229009-24-9P 229009-25-0P
229009-26-1P 229009-27-2P 229009-28-3P 229009-29-4P 229009-30-7P
229009-31-8P 229009-32-9P 229009-33-0P 229009-34-1P 229009-35-2P
229009-36-3P 229009-37-4P 229153-66-6P 229153-67-7P 229153-68-8P
229153-69-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT **229006-01-3P 229006-02-4P 229006-06-8P**
229006-08-0P 229006-12-6P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

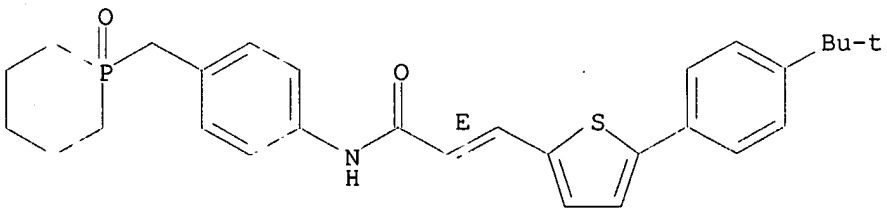
RN 229006-01-3 HCAPLUS
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



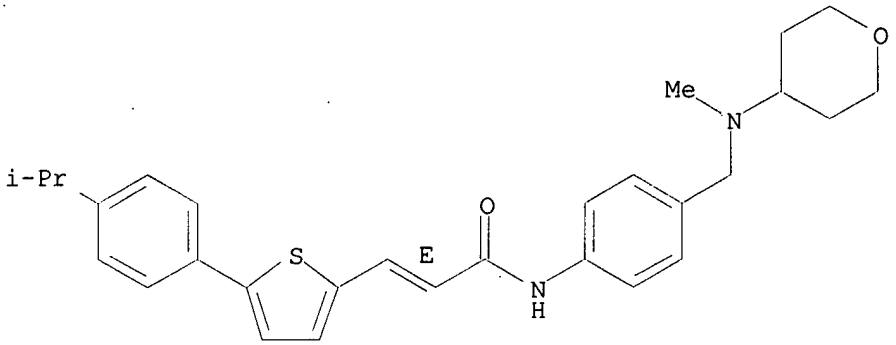
RN 229006-02-4 HCAPLUS
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



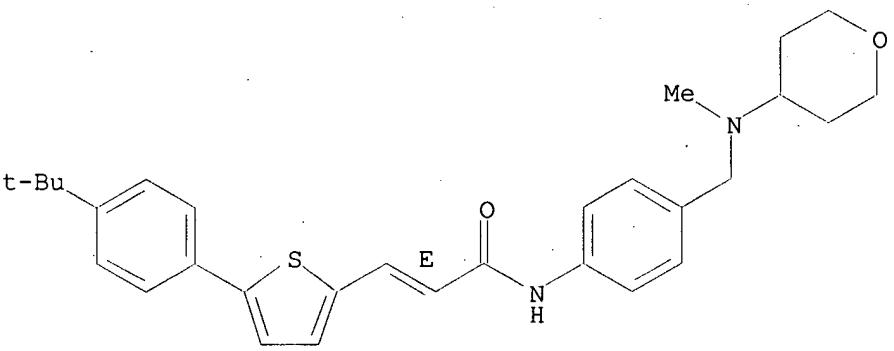
RN 229006-06-8 HCAPLUS
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



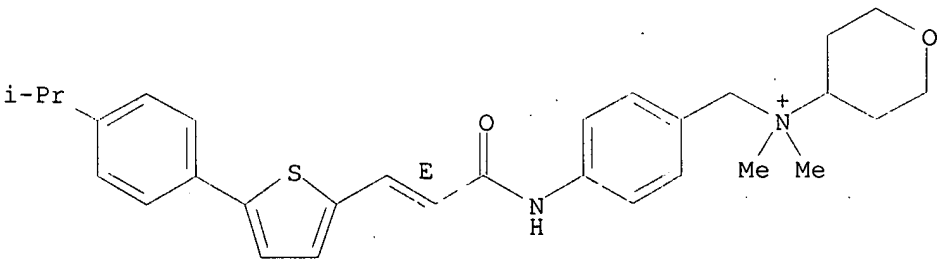
RN 229006-08-0 HCAPLUS
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229006-12-6 HCAPLUS
CN 2H-Pyran-4-aminium, tetrahydro-N,N-dimethyl-N-[[4-[[(2E)-3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-1-oxo-2-propenyl]amino]phenyl]methyl]-, iodide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

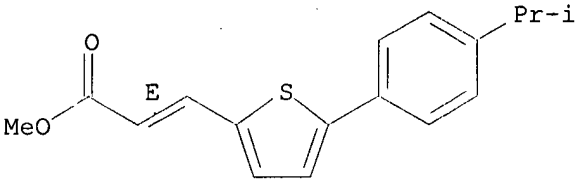


● I^-

IT **229008-54-2P 229008-55-3P 229008-56-4P**
229008-57-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

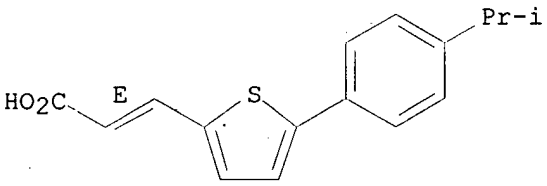
RN 229008-54-2 HCAPLUS
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



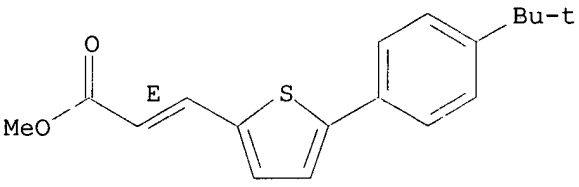
RN 229008-55-3 HCAPLUS
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



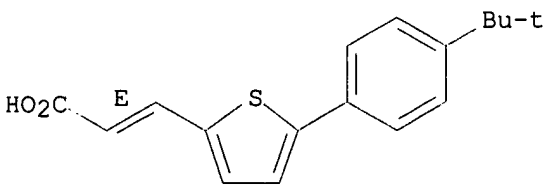
RN 229008-56-4 HCAPLUS
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229008-57-5 HCAPLUS
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L48 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2001 ACS
AN 1997:623162 HCAPLUS
DN 127:293119
TI Preparation of bicyclic aromatic compounds
IN **Bernardon, Jean-Michel**
PA Centre International De Recherches Dermatologiques Galderma (C.I.R.D. Galder, Fr.; Bernardon, Jean-Michel
SO PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DT Patent
LA French
IC ICM C07D333-24
ICS C07D333-16; C07D307-54; C07D207-32; C07D213-55; C07C069-618; A61K031-38; A61K031-19
CC 27-1 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 25, 62, 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO 9733881	A1	19970918	WO 1997-FR391	19970305	<--
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	RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
	FR 2746101	A1	19970919	FR 1996-3235	19960314	<--
	FR 2746101	B1	19980430			
	CA 2218766	AA	19970918	CA 1997-2218766	19970305	<--
	AU 9720305	A1	19971001	AU 1997-20305	19970305	<--
	AU 704753	B2	19990506			
	EP 832081	A1	19980401	EP 1997-908308	19970305	<--
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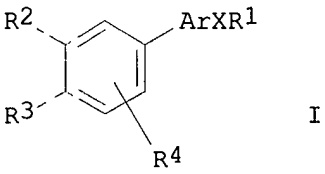
	JP 10509987	T2	19980929	JP 1997-532318	19970305	<--
	JP 2991502	B2	19991220			
	BR 9702200	A	19990720	BR 1997-2200	19970305	<--
	NO 9705192	A	19980114	NO 1997-5192	19971112	<--
	US 6147255	A	20001114	US 1998-952804	19980126	<--
PRAI	FR 1996-3235	A	19960314	<--		
	WO 1997-FR391	W	19970305	<--		

OS MARPAT 127:293119
GI



I

AB Novel bicyclic arom. compds. I [R1 = Me, CH2OR5, COR6; Ar = = (un)substituted Ph, pyridyl, furyl, thienyl, pyrrolyl; X = CR8:CR9, C.tplbond.C; R2, R3 = H, alkyl, OR5, SR5; R2R3 = arom. ring; R5 = H, alkyl, acyl; R6 = H, alkyl, NR'R''; R8, R9 = H, alkyl] and their use in pharmaceutical compns. useful in treatment of dermatol. conditions (no data) or their use in cosmetic compns. (no data) are disclosed. E.g., reaction of 3-tert-butyl-4-methoxyphenylboronic acid and

4-bromo-2-thiophenecarboxaldehyde gave 4-(3-tert-butyl-4-methoxyphenyl)-2-thiophenecarboxaldehyde. The last was treated with tri-Et phosphonoacetate to give Et 4-(3-tert-butyl-4-methoxyphenyl)-2-thiopheneacrylate. The ester was converted to the corresponding acid.

ST bicyclic arom compd prepn; naphthylthiopheneacrylic acid prepn; thiopheneacrylic acid naphthyl prepn; naphthylphenylpropiolic acid prepn; propiolic acid naphthylphenyl prepn; pyrrolylacrylic acid naphthyl prepn; dermatol agent bicyclic arom compd; cosmetic agent bicyclic arom compd

IT Aromatic compounds
RL: BAC (Biological activity or effector, except adverse); BUU (Biological use, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of bicyclic arom. compds.)

IT Cosmetics
(prepn. of bicyclic arom. compds. as cosmetic agents)

IT Skin preparations (pharmaceutical)
(prepn. of bicyclic arom. compds. as dermatol. agents)

IT **196960-59-5P** 196960-60-8P **196960-61-9P**
196960-62-0P 196960-63-1P 196960-64-2P 196960-65-3P
196960-66-4P 196960-67-5P 196960-68-6P 196960-69-7P 196960-70-0P
196960-71-1P 196960-72-2P 196960-73-3P 196960-74-4P 196960-75-5P
196960-76-6P 196960-77-7P 196960-78-8P 196960-79-9P 196960-80-2P
196960-81-3P 196960-82-4P 196960-83-5P 196960-84-6P 196960-85-7P
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196961-50-9P 196961-51-0P 196961-52-1P 196961-53-2P 196961-54-3P
196961-55-4P
RL: BAC (Biological activity or effector, except adverse); BUU (Biological use, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of bicyclic arom. compds.)

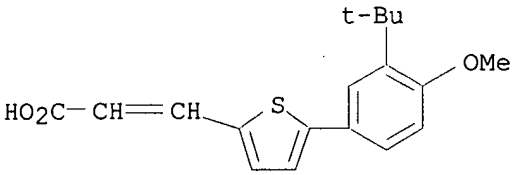
IT 99-90-1 108-40-7, 3-Methylthiophenol 110-91-8, Morpholine, reactions
123-30-8, 4-Hydroxyaniline 629-04-9, 1-Bromoheptane 870-63-3
931-33-9 1122-91-4, 4-Bromobenzaldehyde 1200-07-3 1761-61-1,
5-Bromo-2-hydroxybenzaldehyde 4701-17-1 14804-34-3 18791-75-8
27452-17-1 62224-19-5 119999-22-3 168082-64-2 170355-38-1
RL: RCT (Reactant)
(prepn. of bicyclic arom. compds.)

IT 33694-79-0P 135631-86-6P 158115-92-5P 168082-41-5P 169126-63-0P
169126-64-1P 170100-73-9P 189698-90-6P 189698-91-7P 189699-37-4P
191469-48-4P 196960-90-4P 196960-91-5P 196960-92-6P 196960-93-7P
196960-94-8P **196960-95-9P** 196960-96-0P 196960-97-1P
196960-98-2P 196960-99-3P **196961-00-9P** 196961-01-0P
196961-02-1P 196961-03-2P 196961-04-3P 196961-05-4P
196961-06-5P 196961-07-6P 196961-08-7P 196961-09-8P 196961-10-1P
196961-11-2P 196961-12-3P 196961-13-4P 196961-14-5P 196961-15-6P
196961-16-7P 196961-17-8P 196961-18-9P 196961-19-0P 196961-20-3P
196961-21-4P 196961-22-5P 196961-23-6P 196961-24-7P 196961-25-8P
196961-26-9P 196961-27-0P 196961-28-1P 196961-29-2P 196961-30-5P
196961-31-6P 196961-32-7P 196961-33-8P 196961-34-9P 196961-35-0P
196961-36-1P 196961-37-2P 196961-38-3P 196961-39-4P 196961-40-7P
196961-41-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of bicyclic arom. compds.)

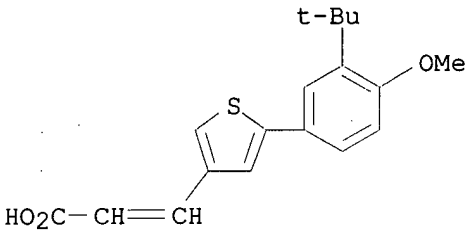
IT **196960-59-5P 196960-61-9P 196960-62-0P**
RL: BAC (Biological activity or effector, except adverse); BUU (Biological use, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of bicyclic arom. compds.)

RN 196960-59-5 HCAPLUS

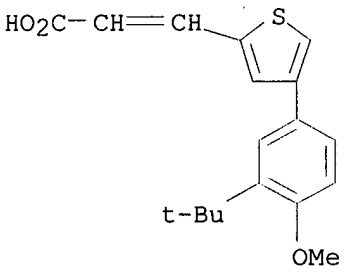
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]-(9CI) (CA INDEX NAME)



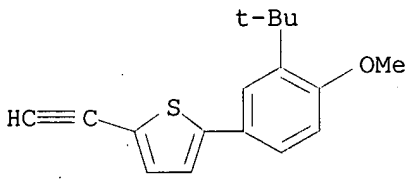
RN 196960-61-9 HCAPLUS
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]- (9CI) (CA INDEX NAME)



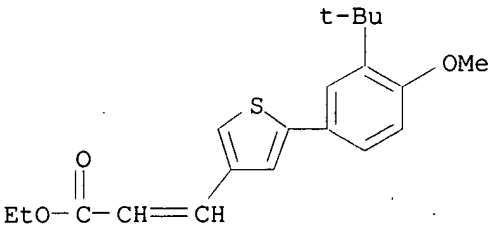
RN 196960-62-0 HCAPLUS
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]- (9CI) (CA INDEX NAME)



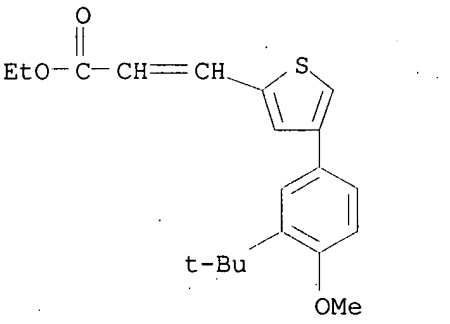
IT **196960-95-9P 196961-00-9P 196961-02-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of bicyclic arom. compds.)
RN 196960-95-9 HCAPLUS
CN Thiophene, 2-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-5-ethynyl- (9CI) (CA INDEX NAME)



RN 196961-00-9 HCAPLUS
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)

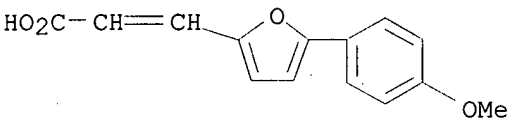


RN 196961-02-1 HCAPLUS
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)

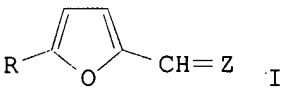


L48 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2001 ACS
AN 1997:131476 HCAPLUS
DN 126:238323
TI Synthesis of 2-arylfuro[3,2-c]pyridines and their derivatives
AU Krutosikova, Alzbeta; Sleziak, Robert
CS Department of Organic Chemistry, Slovak Technical University, Bratislava, 812 37, Slovakia
SO Collect. Czech. Chem. Commun. (**1996**), 61(11), 1627-1636
CODEN: CCCCAK; ISSN: 0010-0765
PB Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
DT Journal
LA English
CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))
AB A series of 2-arylfuro[3,2-c]pyridines was synthesized. 3-(5-Aryl-2-furyl)propenoic acids were converted to the acid azides, which in turn were cyclized to give 2-arylfuro[3,2-c]pyridine-4(5H)-ones 4 by heating in Dowtherm. The pyridones 4 were aromatized with phosphorus oxychloride to the 2-aryl-4-chlorofuro[3,2-c]pyridines, which were reduced with zinc and acetic acid to the title compds. Reacted with phosphorus(V) sulfide, the pyridones 4 yielded the corresponding thiones.
ST furopyridine aryl prepn; cyclization furylpropenoate
IT Cyclization
(of furylpropenoates)
IT 63731-38-4P 188437-94-7P 188437-95-8P 188437-96-9P 188437-97-0P 188437-98-1P 188437-99-2P 188438-00-8P 188438-01-9P 188438-02-0P 188438-03-1P 188438-04-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 141-82-2, Malonic acid, reactions 7147-77-5, 5-(4-Nitrophenyl)furfural 13148-43-1, 5-(3-Nitrophenyl)furfural 13803-39-9, 5-Phenylfurfural 20005-42-9, 5-(4-Bromophenyl)furfural 34035-03-5, 5-(4-Chlorophenyl)furfural 34035-05-7, 5-(4-Methylphenyl)furfural 34070-33-2, 5-(4-Methoxyphenyl)furfural 52130-34-4, 5-(3,4-Dichlorophenyl)furfural
RL: RCT (Reactant)

(synthesis of 2-arylfuro[3,2-c]pyridines and their derivs.)
IT 58110-34-2P 58110-35-3P 58110-37-5P 58110-40-0P 58110-42-2P
58110-43-3P **58110-44-4P** 179870-08-7P 179870-09-8P
188437-73-2P 188437-74-3P 188437-75-4P 188437-76-5P 188437-77-6P
188437-78-7P 188437-80-1P 188437-81-2P 188437-82-3P 188437-83-4P
188437-84-5P 188437-85-6P 188437-86-7P 188437-87-8P 188437-88-9P
188437-89-0P 188437-90-3P 188437-91-4P 188437-92-5P 188437-93-6P
188438-05-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 2-arylfuro[3,2-c]pyridines and their derivs.)
IT **58110-44-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 2-arylfuro[3,2-c]pyridines and their derivs.)
RN 58110-44-4 HCAPLUS
CN 2-Propenoic acid, 3-[5-(4-methoxyphenyl)-2-furanyl]- (9CI) (CA INDEX NAME)



L48 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2001 ACS
AN 1990:552173 HCAPLUS
DN 113:152173
TI Arylation of furanoid compounds with aryldiazonium salts
AU Obushak, N. D.; Ganushchak, N. I.; Lesyuk, A. I.; Dzikovskaya, L. M.; Kisilitsa, P. P.
CS L'vov. Gos. Univ., Lvov, USSR
SO Zh. Org. Khim. (**1990**), 26(4), 873-80
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
OS CASREACT 113:152173
GI

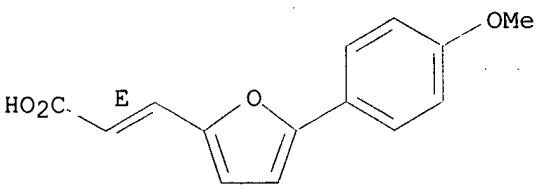


I

AB Condensation reaction of arylfurfurals I (R = Ph, 4-MeOC6H4, 4-ClC6H4, 4-O2NC6H4, 2- and 4-BrC6H4, 4-tolyl, 1-naphthyl; Z = O) with CH2(CO2H)2 in refluxing pyridine contg. piperidine gave 58-92% furylacrylic acids I (Z = CHCO2H-E), which were arylated with R1N2+ Cl- (R1 = Ph, 4-ClC6H4, 2- and 4-BrC6H4, 4-O2NC6H4, 4-EtO2CC6H4) in aq. Me2CO contg. NaOAc and CuCl2 to 8 I (Z = CHR1-E) (II) in 27-54% yield. II were also prepd. in 16-40% yield along with 17-32% I (Z = CHO-E) by arylating 3-(2-furyl)acrolein as above. I (R = Ph, 4-ClC6H4; Z = CHCHO-E) were also formed in 40-50% yield by treating I (Z = O) with MeCHO in H2O-CH2Cl2 contg. NaOH and BuNEt3+ Cl-.
ST arylation furan deriv diazonium salt; styrylfuran furylacrolein prepn UV NMR; furylacrylic acid prepn arylation; acrylic acid furyl prepn arylation; acrolein furyl prepn UV NMR
IT Nuclear magnetic resonance
Ultraviolet and visible spectra
(of (arylfuryl)acroleins and arylstyrylfurans)
IT Arylation
(of furanoid compds. with aryldiazonium salts)
IT Diazonium compounds
RL: RCT (Reactant)

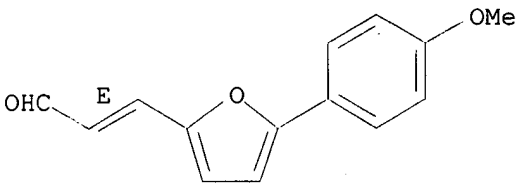
(arene, salts, arylation by, of furanoid compds.)
IT 2028-79-7, 4-(Ethoxycarbonyl)phenyldiazonium chloride 2028-85-5, 4-Bromophenyldiazonium chloride
RL: RCT (Reactant)
(arylation by, of (arylfuryl)acrylic acids)
IT 100-05-0 100-34-5 2028-74-2, 4-Chlorophenyldiazonium chloride 4346-59-2, 4-Methoxyphenyldiazonium chloride 34835-57-9, 2-Bromophenyldiazonium chloride
RL: RCT (Reactant)
(arylation by, of furylacrolein and (arylfuryl)acrylic acids)
IT 623-30-3, 3-(2-Furyl)acrolein
RL: RCT (Reactant)
(arylation of, with aryldiazonium chlorides)
IT 75-07-0, Acetaldehyde, reactions
RL: RCT (Reactant)
(condensation reaction of, with arylfurfurals, (arylfuryl)acroleins by)
IT 141-82-2, Propanedioic acid, reactions
RL: RCT (Reactant)
(condensation reaction of, with arylfurfurals, (arylfuryl)acrylic acids by)
IT 7147-77-5, 5-(4-Nitrophenyl)furfural 13803-39-9, 5-Phenylfurfural 20005-42-9, 5-(4-Bromophenyl)furfural 34035-03-5, 5-(4-Chlorophenyl)furfural 34035-05-7, 5-(4-Tolyl)furfural 34070-33-2, 5-(4-Methoxyphenyl)furfural 51792-36-0 58110-57-9, 5-(2-Bromophenyl)furfural
RL: RCT (Reactant)
(condensation reaction of, with malonic acid, (arylfuryl)acrylic acid by)
IT **62806-31-9P** 62806-32-0P 62806-33-1P 62806-34-2P 62806-35-3P 62806-39-7P 129626-52-4P 129626-62-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and arylation of, with aryldiazonium salts)
IT 40025-25-0P 104431-32-5P 108576-24-5P 129626-53-5P 129626-54-6P 129626-55-7P 129626-56-8P 129626-57-9P 129626-58-0P **129626-59-1P** 129626-60-4P 129626-61-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **62806-31-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and arylation of, with aryldiazonium salts)
RN 62806-31-9 HCAPLUS
CN 2-Propenoic acid, 3-[5-(4-methoxyphenyl)-2-furanyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

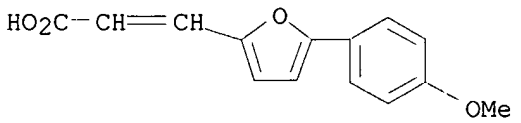


IT **129626-59-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 129626-59-1 HCAPLUS
CN 2-Propenal, 3-[5-(4-methoxyphenyl)-2-furanyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

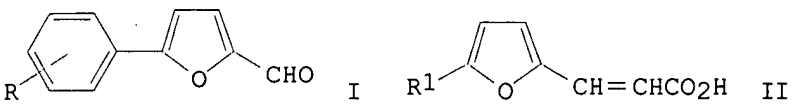


L48 ANSWER 7 OF 10 HCAPLUS COPYRIGHT 2001 ACS
AN 1988:510184 HCAPLUS
DN 109:110184
TI Synthesis of substituted furylacrylic acids and their chlorides
AU Lesyuk, A. I.; Dzikovskaya, L. M.; Obushak, N. D.; Ganushchak, N. I.
CS USSR
SO Vestn. L'vov. Un-ta. Ser. Khim. (**1987**), (28), 82-6
From: Ref. Zh., Khim. 1987, Abstr. No. 22Zh168
DT Journal
LA Russian
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
AB Title only translated.
ST arylfurfuryl alc Knoevenagel condensation malonate; furylacrylic acid prepn chlorination; furylacryloyl chloride
IT Knoevenagel reaction
(of arylfurfuryl alcs. with malonic acid, furylacrylic acid by)
IT 141-82-2, Malonic acid, reactions
RL: RCT (Reactant)
(Knoevenagel reaction of, with arylfurfuryl alcs.)
IT 7147-77-5 13803-39-9 20005-42-9 34035-03-5 34035-05-7 34070-33-2 58110-57-9
RL: RCT (Reactant)
(Knoevenagel reaction of, with malonic acid)
IT 58110-37-5P 58110-42-2P 58110-43-3P **58110-44-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion of, to acid chloride)
IT 58110-34-2P 58110-40-0P 58110-41-1P 116218-06-5P 116218-07-6P 116218-08-7P 116218-09-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **58110-44-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion of, to acid chloride)
RN 58110-44-4 HCAPLUS
CN 2-Propenoic acid, 3-[5-(4-methoxyphenyl)-2-furanyl]- (9CI) (CA INDEX NAME)

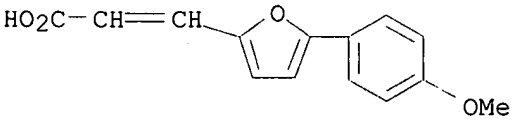


L48 ANSWER 8 OF 10 HCAPLUS COPYRIGHT 2001 ACS
AN 1987:534142 HCAPLUS
DN 107:134142
TI Catalytic arylation of furfural with arenediazonium salts
AU Obushak, N. D.; Lesyuk, A. I.; Ganushchak, N. I.; Mel'nik, G. M.; Zavalii, P. Yu.
CS L'vov. Gos. Univ., Lvov, USSR
SO Zh. Org. Khim. (**1986**), 22(11), 2331-6
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal

LA Russian
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
OS CASREACT 107:134142
GI



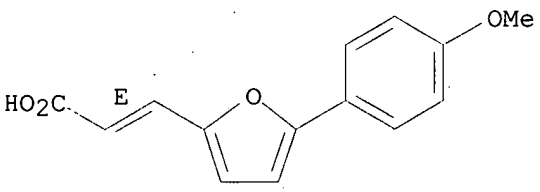
AB Arylfurfurals I (R = H, 2-, 3-, 4-Me, 2,4-Me2, 2-, 4-MeO, 4-EtO, 3-Br, 4-iodo) were prepd. in 12-50% yields by arylation of furfural with benzene diazonium chlorides in aq. Me2CO contg. CuCl2.2H2O or FeCl2.4H2O. Similarly, treating arylfurfurals with CH2(CO2H)2 gave 70 and 63% furanacrylic acids II (R1 = Ph, 4-MeOC6H4).
ST arylation catalytic furfural benzenediazonium
IT Arylation catalysts
(cupric chloride, for furfural by arene diazonium salts)
IT Arylation
(of furfural by arenediazonium salts in presence of cupric chloride)
IT Diazonium compounds
RL: RCT (Reactant)
(arene, arylation of furfural by)
IT 100-34-5, Benzenediazonium chloride 2028-34-4, 2-Methylbenzenediazonium chloride 2028-72-0, 3-Methylbenzenediazonium chloride 2028-84-4, 4-Methylbenzenediazonium chloride 3177-49-9 3425-23-8, 2-Methoxybenzenediazonium chloride 4346-59-2, 4-Methoxybenzenediazonium chloride 16048-37-6 20893-72-5, 4-Iodobenzenediazonium chloride 20893-74-7, 3-Bromobenzenediazonium chloride 20893-80-5 36968-72-6 38793-99-6, 4-Ethoxybenzenediazonium chloride 53559-94-7
RL: RCT (Reactant)
(arylation by, of furfural)
IT 98-01-1, Furfural, reactions
RL: RCT (Reactant)
(catalytic arylation of, by arenediazonium salts)
IT 13803-39-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with malonic acid)
IT 34035-05-7P 34070-33-2P 39868-10-5P 51792-36-0P 51792-37-1P 58110-42-2P **58110-44-4P** 64251-78-1P 94078-19-0P 94078-20-3P 99142-57-1P 110360-09-3P 110360-10-6P 110360-11-7P 110360-12-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **58110-44-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 58110-44-4 HCAPLUS
CN 2-Propenoic acid, 3-[5-(4-methoxyphenyl)-2-furanyl]- (9CI) (CA INDEX NAME)



L48 ANSWER 9 OF 10 HCAPLUS COPYRIGHT 2001 ACS
AN 1977:188948 HCAPLUS
DN 86:188948
TI Transmission of substituent effects across the furan ring

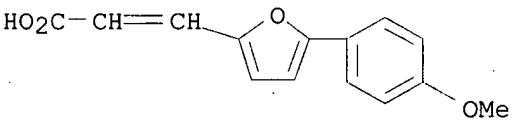
AU Beno, A.; Krutosikova, A.
CS Dep. Anal. Chem., Comenius Univ., Bratislava, Czech.
SO Collect. Czech. Chem. Commun. (**1977**), 42(2), 508-11
CODEN: CCCCAK
DT Journal
LA English
CC 22-8 (Physical Organic Chemistry)
AB The half-wave potential values, apparent dissocn. consts., and wavenos. of IR bands of 9 substituted 3-(5-phenyl-2-furyl)acrylic acids and 8 substituted cinnamic acids were correlated with .sigma. substituent consts. The transmission coeffs. across the furan ring, .pi.', were calcd. from the obtained reaction consts. .rho. and compared with the values of .pi.' found for other systems. There was good agreement between the results obtained by different methods., and between the present and previous results (Beno, A., et al., 1973).
ST furanacrylic acid Hammett LFER; cinnamic acid Hammett LFER; acid cinnamic furanacrylic Hammett; substituent cinnamic furanacrylic acid; IR cinnamic furanacrylic acid; polarog cinnamic furanacrylic acid
IT Dissociation
Infrared spectra
Polarography
(of furyl- and phenylacrylic acids)
IT Substituent effect
(on properties of cinnamic and furanacrylic acids)
IT Linear free energy relationship
(Hammett, of furyl- and phenylacrylic acids)
IT 940-61-4 940-62-5 7312-27-8 14473-90-6 14737-89-4 17570-26-2 20595-30-6 **62806-31-9** 62806-32-0 62806-33-1 62806-34-2 62806-35-3 62806-37-5 62806-38-6
RL: PRP (Properties)
(dissocn., polarog., and IR of, Hammett relationship of)
IT 140-10-3, reactions
RL: RCT (Reactant)
(dissocn., polarog., and IR of, Hammett relationshp of)
IT 62806-36-4 62806-39-7
RL: PRP (Properties)
(dissocn., polarog.,and IR of, Hammett relationship of)
IT **62806-31-9**
RL: PRP (Properties)
(dissocn., polarog., and IR of, Hammett relationship of)
RN 62806-31-9 HCAPLUS
CN 2-Propenoic acid, 3-[5-(4-methoxyphenyl)-2-furanyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

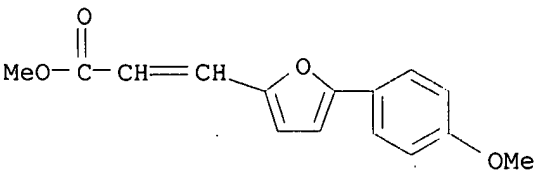


L48 ANSWER 10 OF 10 HCAPLUS COPYRIGHT 2001 ACS
AN 1976:58390 HCAPLUS
DN 84:58390
TI Furan derivatives. LXIII. Substituted 3-(5-phenyl-2-furyl)acrylic acids and their methyl esters. Transmission of polar effects across the furan-ethene system
AU Krutosikova, A.; Sura, J.; Kovac, J.; Juhas, S.
CS Dep. Org. Chem., Slovak Inst. Technol., Bratislava, Czech.
SO Collect. Czech. Chem. Commun. (**1975**), 40(11), 3362-9
CODEN: CCCCAK

DT Journal
LA English
CC 22-8 (Physical Organic Chemistry)
AB Thirteen 3-(5-phenyl-2-furyl)acrylic acids (unsubstituted or substituted by NO2, Cl, Br, Me, MeO, or CF3) were prepd. by Perkin condensation of the corresponding furancarboxaldehydes. The apparent pKa values of the acids in 80% methyl cellosolve and the rate consts. kh of the alk. hydrolysis of their Me esters in 60% aq. Me2CO were detd. potentiometrically. The obtained values are correlated with .sigma. substituent consts. and the transmission of the polar effects of the substituents across the furan-ethene system is discussed.
ST phenylfuranacrylic acid dissocn const; hydrolysis const phenylfuranacrylate; polar effect phenylfuranacrylate; Hammet phenylfuranacrylate; furanacrylate phenyl polar effect; acrylate phenylfuryl polar effect
IT Dissociation
(consts., of phenylfuranacrylic acids)
IT Kinetics of hydrolysis
(of methyl phenylfuranacrylates)
IT Substituent effect
(on dissocn. of phenylfuranacrylic acids or hydrolysis of their methyl esters)
IT 7147-77-5 13148-43-1 13803-39-9 20000-96-8 20005-42-9 22078-59-7 34035-03-5 34035-04-6 34035-05-7 34070-33-2 52130-30-0 58110-57-9 58110-58-0
RL: RCT (Reactant)
(Perkin reaction of)
IT 58110-34-2P 58110-35-3P 58110-36-4P 58110-37-5P 58110-38-6P 58110-39-7P 58110-40-0P 58110-41-1P 58110-42-2P 58110-43-3P **58110-44-4P** 58110-45-5P 58110-46-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and dissocn. const. of)
IT 58110-47-7P 58110-48-8P 58110-49-9P 58110-50-2P 58110-51-3P 58110-52-4P 58110-53-5P 58110-54-6P **58110-55-7P** 58110-56-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis const. of)
IT **58110-44-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and dissocn. const. of)
RN 58110-44-4 HCAPLUS
CN 2-Propenoic acid, 3-[5-(4-methoxyphenyl)-2-furanyl]- (9CI) (CA INDEX NAME)



IT **58110-55-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis const. of)
RN 58110-55-7 HCAPLUS
CN 2-Propenoic acid, 3-[5-(4-methoxyphenyl)-2-furanyl]-, methyl ester (9CI) (CA INDEX NAME)



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CA INDEXING COPYRIGHT (C) 2001 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 5 Jul 2001 (20010705/PD)
FILE LAST UPDATED: 5 Jul 2001 (20010705/ED)
HIGHEST GRANTED PATENT NUMBER: US6249914
HIGHEST APPLICATION PUBLICATION NUMBER: US2001007157
CA INDEXING IS CURRENT THROUGH 5 Jul 2001 (20010705/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 5 Jul 2001 (20010705/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2001
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2001

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>>> Page images are available for display by the following day.     <<<
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>>> is included in file records. A thesaurus is available for the  <<<
>>> USPTO Manual of Classifications in the /NCL, /INCL, and /RPCL  <<<
>>> fields. This thesaurus includes catchword terms from the       <<<
>>> USPTO/MOC subject headings and subheadings. Thesauri are also  <<<
>>> available for the WIPO International Patent Classification     <<<
>>> (IPC) Manuals, editions 1-6, in the /IC1, /IC2, /IC3, /IC4,    <<<
>>> /IC5, and /IC (/IC6) fields, respectively. The thesauri in     <<<
>>> the /IC5 and /IC fields include the corresponding catchword    <<<
>>> terms from the IPC subject headings and subheadings.           <<<

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> d bib abs hitstr tot l49

L49  ANSWER 1 OF 3  USPATFULL
AN     2000:174633  USPATFULL
TI     Anilide derivative, production and use thereof
IN     Shiraishi, Mitsuru, Hyogo, Japan
       Kitayoshi, Takahito, Osaka, Japan
       Aramaki, Yoshio, Hyogo, Japan
       Honda, Susumu, Hyogo, Japan
       Oda, Tsuneo, Osaka, Japan
PA     Takeda Chemical Industries, Ltd., Osaka, Japan (non-U.S. corporation)
PI     US 6166006  20001226
AI     US 1998-213379  19981217 (9)
PRAI   JP 1997-351481      19971219
DT     Utility
EXNAM  Primary Examiner: Powers, Fiona T.
LREP   Wenderoth, Lind & Ponack, L.L.P.
CLMN   Number of Claims: 26
ECL    Exemplary Claim: 1
DRWN   No Drawings
LN.CNT 15554
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB     This invention is to provide a compound of the formula: ##STR1## wherein
       R.sup.1 is an optionally substituted 5- to 6-membered ring: C is a
       divalent group of the formula: ##STR2## wherein the ring A is an
       optionally substituted 5- to 6-membered aromatic ring, X is an
       optionally substituted C, N or O atom, and the ring B is an optionally
       substituted 5- to 7-membered ring; Z is a chemical bond or a divalent
       group; R.sup.2 is (1) an optionally substituted amino group in which a
       nitrogen atom may form a quaternary ammonium, etc., or a salt thereof,
       which is useful for antagonizing MCP-1 receptor.
```

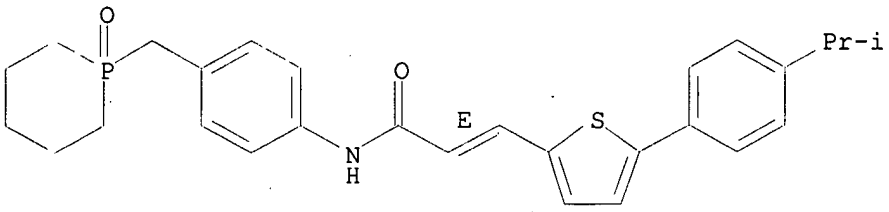
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **229006-01-3P 229006-02-4P 229006-06-8P**
229006-08-0P 229006-12-6P
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

RN 229006-01-3 USPATFULL

CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

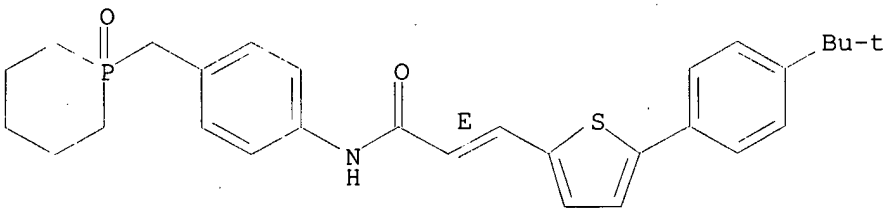
Double bond geometry as shown.



RN 229006-02-4 USPATFULL

CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

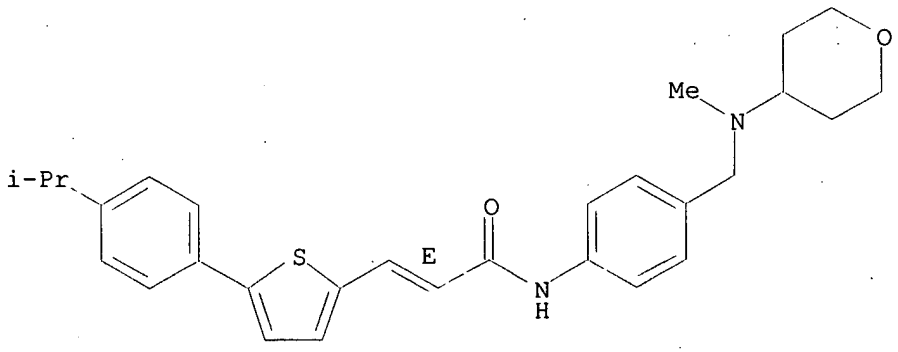
Double bond geometry as shown.



RN 229006-06-8 USPATFULL

CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

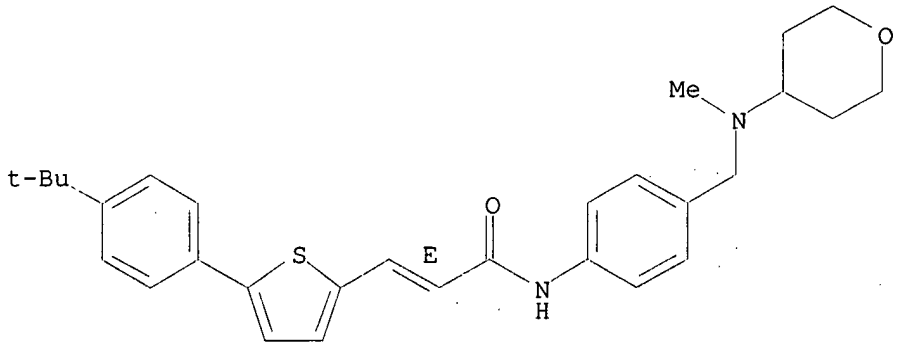
Double bond geometry as shown.



RN 229006-08-0 USPATFULL

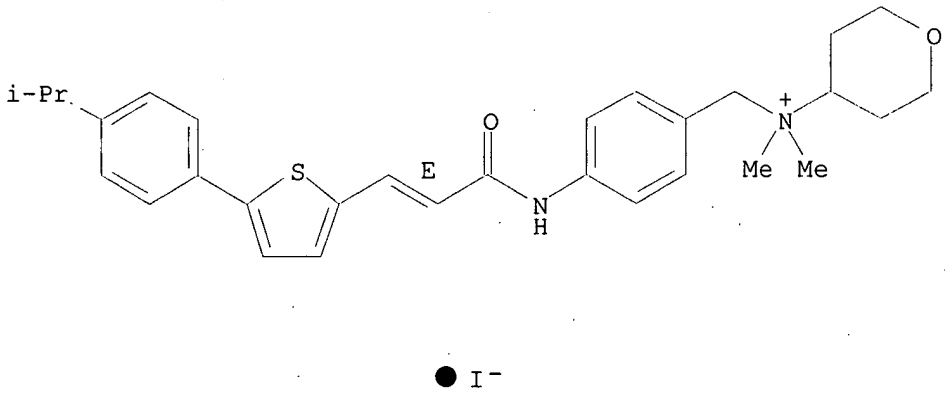
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229006-12-6 USPATFULL
CN 2H-Pyran-4-aminium, tetrahydro-N,N-dimethyl-N-[[4-[[(2E)-3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-1-oxo-2-propenyl]amino]phenyl]methyl]-, iodide (9CI) (CA INDEX NAME)

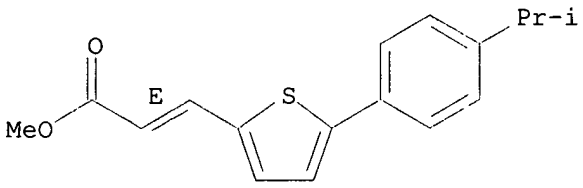
Double bond geometry as shown.



● I^-

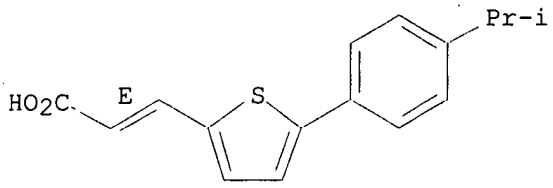
IT **229008-54-2P 229008-55-3P 229008-56-4P 229008-57-5P**
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)
RN 229008-54-2 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



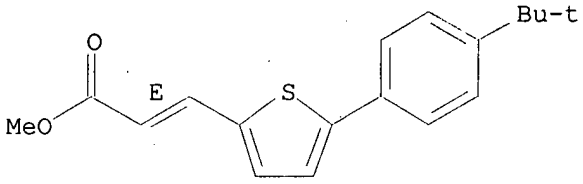
RN 229008-55-3 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



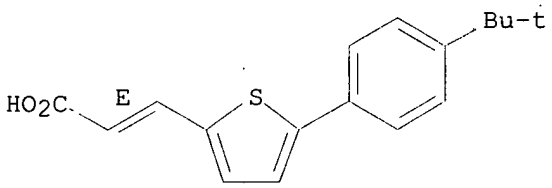
RN 229008-56-4 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229008-57-5 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

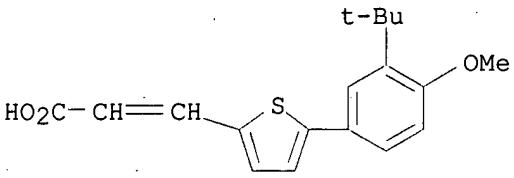
Double bond geometry as shown.



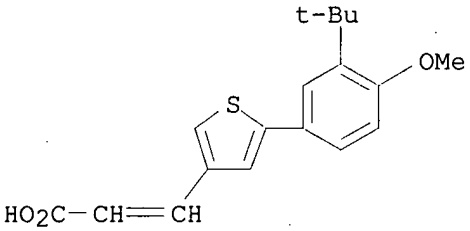
L49 ANSWER 2 OF 3 USPATFULL
AN 2000:153887 USPATFULL
TI Bicyclic-aromatic compounds
IN Bernardon, Jean-Michel, Le Rouret, France
PA Centre International de Recherches Dermatologiques Galderma, Valbonne, France (non-U.S. corporation)
PI US 6147255 20001114
WO 9733881 19970918
AI US 1998-952804 19980126 (8)
WO 1997-FR391 19970305
19980126 PCT 371 date
19980126 PCT 102(e) date
PRAI FR 1996-3235 19960314
DT Utility
EXNAM Primary Examiner: Oazi, Sabiha
LREP Burns, Doane, Swecker & Mathis, L.L.P.
CLMN Number of Claims: 10
ECL Exemplary Claim: 1
DRWN 1 Drawing Figure(s); 1 Drawing Page(s)
LN.CNT 1471
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The invention relates to novel bicyclic aromatic compounds which have the general formula (I): ##STR1## as well as to the use of these compounds in pharmaceutical compositions intended for use in human or veterinary medicine (dermatological, rheumatic, respiratory,

cardiovascular and ophthalmological complaints in particular), or alternatively in cosmetic compositions.

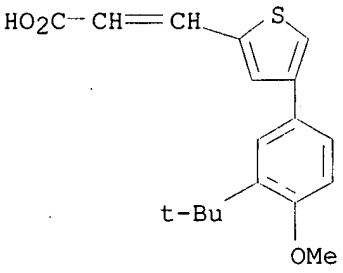
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **196960-59-5P 196960-61-9P 196960-62-0P**
(prepn. of bicyclic arom. compds.)
RN 196960-59-5 USPATFULL
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]- (9CI) (CA INDEX NAME)



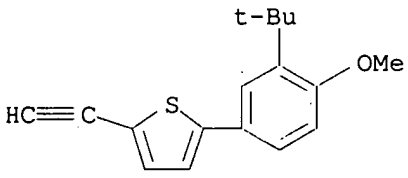
RN 196960-61-9 USPATFULL
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]- (9CI) (CA INDEX NAME)



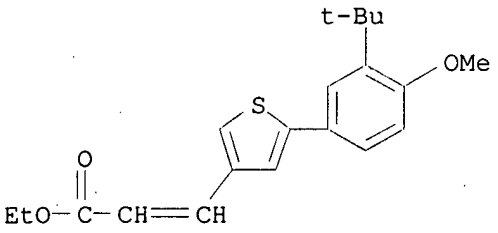
RN 196960-62-0 USPATFULL
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]- (9CI) (CA INDEX NAME)



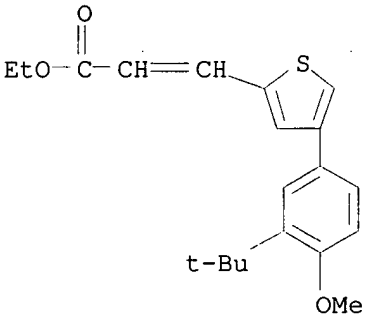
IT **196960-95-9P 196961-00-9P 196961-02-1P**
(prepn. of bicyclic arom. compds.)
RN 196960-95-9 USPATFULL
CN Thiophene, 2-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-5-ethynyl- (9CI) (CA INDEX NAME)



RN 196961-00-9 USPATFULL
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 196961-02-1 USPATFULL
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



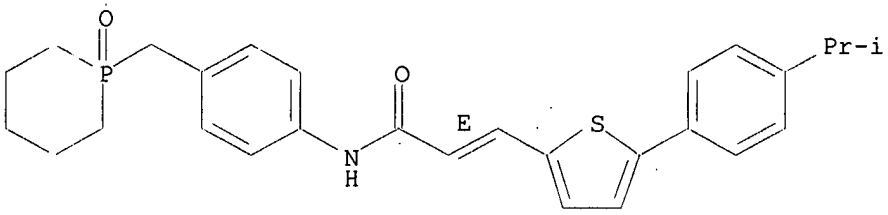
L49 ANSWER 3 OF 3 USPATFULL
AN 2000:98464 USPATFULL
TI Quaternary ammonium salts and their use
IN Shiraishi, Mitsuru, Hyogo, Japan
Baba, Masanori, Kagoshima, Japan
Aramaki, Yoshio, Hyogo, Japan
Nishimura, Osamu, Ibaraki, Japan
Kanzaki, Naoyuki, Osaka, Japan
PA Takeda Chemical Industries, Ltd., Osaka, Japan (non-U.S. corporation)
PI US 6096780 20000801
AI US 1999-377040 19990819 (9)
PRAI JP 1998-234388 19980820
US 1998-104845 19981016 (60)
DT Utility
EXNAM Primary Examiner: Lambkin, Deborah C.
LREP Wenderoth, Lind & Ponack, LLP.
CLMN Number of Claims: 22
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 2169
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB This invention is to provide a compound for antagonizing CCR5, said compound being represented by the formula: ##STR1## wherein R.sup.1 is an optionally substituted phenyl or an optionally substituted thienyl; Y is --CH.sub.2 --, --S-- or --O--; and R.sup.2, R.sup.3 and R.sup.4 are independently an optionally substituted aliphatic hydrocarbon group or an optionally substituted alicyclic heterocyclic ring group, and being effective for the prevention and treatment of infectious disease of HIV.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **229006-01-3P 229006-02-4P 229006-06-8P 229006-08-0P 229006-12-6P**

(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

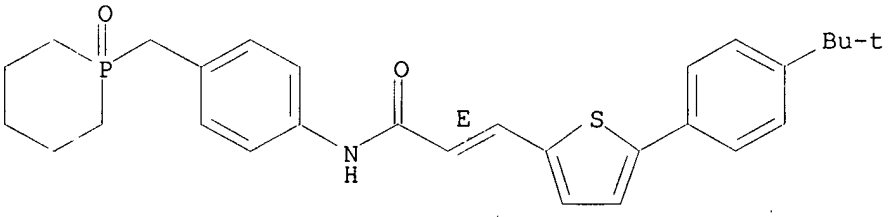
RN 229006-01-3 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



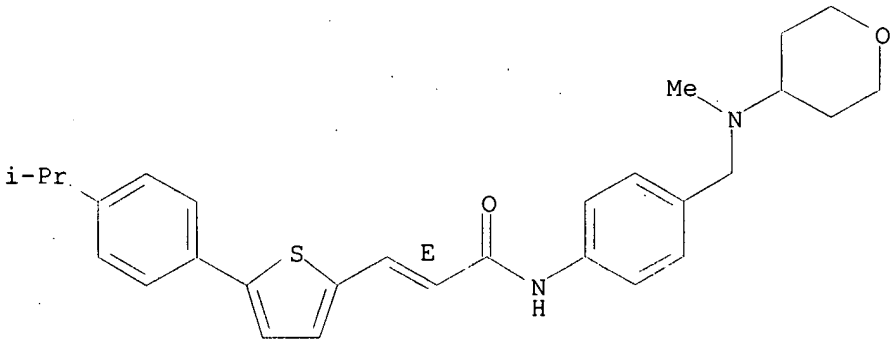
RN 229006-02-4 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



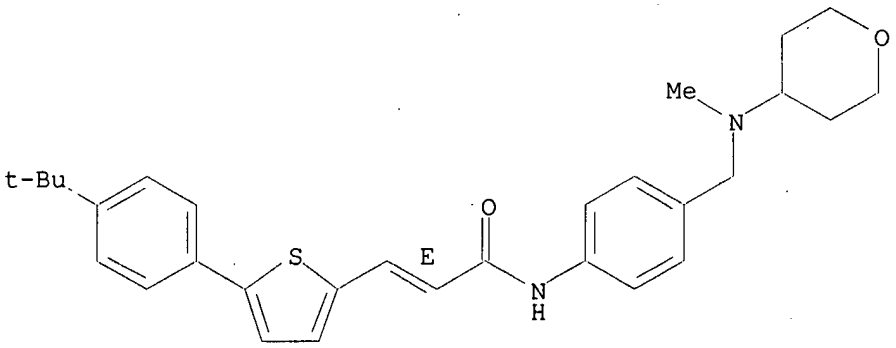
RN 229006-06-8 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



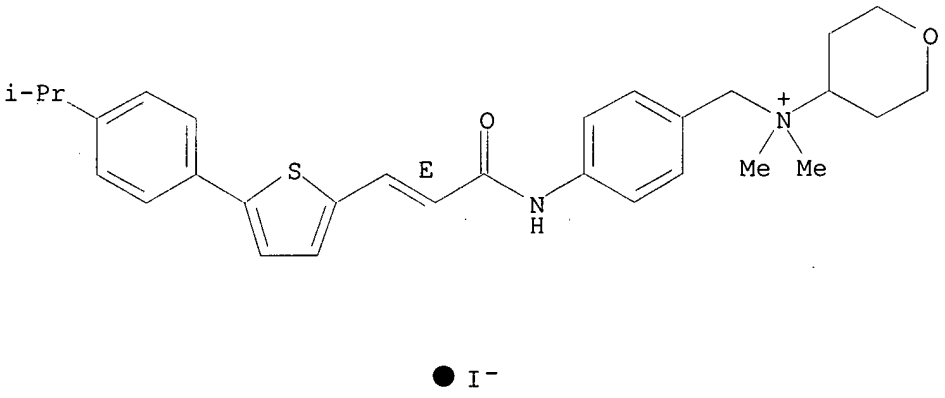
RN 229006-08-0 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229006-12-6 USPATFULL
CN 2H-Pyran-4-aminium, tetrahydro-N,N-dimethyl-N-[[4-[[(2E)-3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-1-oxo-2-propenyl]amino]phenyl]methyl]-, iodide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

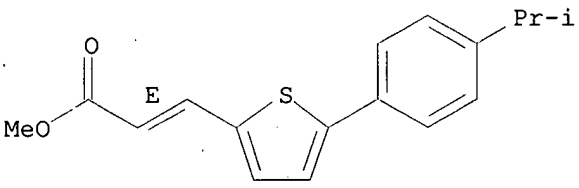


● I^-

IT **229008-54-2P 229008-55-3P 229008-56-4P**
229008-57-5P
(prepn. of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

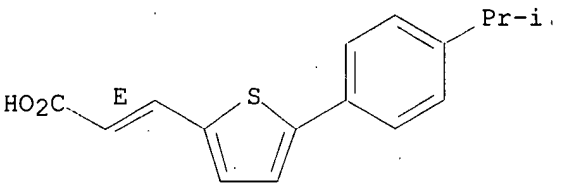
RN 229008-54-2 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



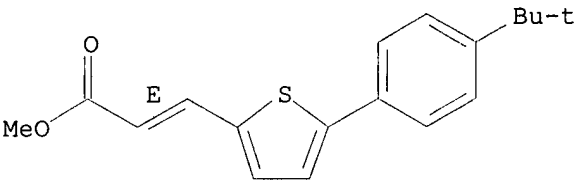
RN 229008-55-3 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229008-56-4 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229008-57-5 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.